
dipc2016
Donostia International Physics Center

ON THE COVER **SALOL**

BY DAVID MAITLAND

An early anticeptic, phenyl salicylate, or salol, was discovered in 1886 by heating salicylic acid with phenol. Once used in sunscreens, phenyl salicylate is now used in the manufacture of some polymers, lacquers, adhesives, waxes and polishes. Schools use it to demonstrate how cooling rates affect crystal size in igneous rocks. It also has a useful antibacterial activity within the small intestine and is a mild painkiller.

2016

DIPC ACTIVITY REPORT

DIPC: a World of Science, Science in the World

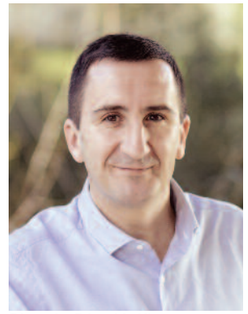
Donostia International Physics Center (DIPC) is a research center that started activity in the year 2000. Promoted and funded by public institutions (Department of Education and Department of Economic Development of Basque Government, Provincial Authority of Gipuzkoa, San Sebastian Town Hall, University of the Basque Country) and private companies (currently Kutxa, CAF, Telefónica, and EDP), DIPC is singular both in its institutional structure and in its flexible way of operation.

The main goal of DIPC is to generate new knowledge at the frontiers of physics and related fields. Since its creation, DIPC has been an open institution that welcomes visitors from all over the world, cultivates the free exchange of ideas, and fosters a generous collaboration among scientists.

The intellectual environment at DIPC leads to an exciting atmosphere that stimulates the creativity and performance of all researchers.

For many years, the core of DIPC scientific activity was mostly focused on some aspects of condensed matter physics and materials sciences. The recent growth of DIPC activity, however, has been accompanied by an expansion of topics and research interests. A great part of this expansion has been pushed by the attraction of researchers hired through the Basque Agency for Science, Ikerbasque, which have complemented and enriched an already excellent community of researchers. Scientists at DIPC currently work on a large collection of topics, including advanced materials, attophysics, surfaces and interfaces, photonics, plasmonics, quantum information, polymers, soft matter, biofunctional nanosystems, computational chemistry, etc. We anticipate that this large variety of research lines will do nothing but grow in the near future, spurring the multidisciplinary view of research that characterizes the center.

DIPC encompasses a wondrous world of science within its walls.



Ricardo Díez Muiño
Director

At DIPC, we are convinced of the cultural, social, and economical worth of science. And we are also convinced of the necessity of moving science from academic environments to mainstream society, to the world. The scientific adventure needs to be prompted and enjoyed by all citizens. For this reason, and in addition to its scientific research, DIPC holds an intense activity in the public dissemination of science, including programs such as *Kutxa Lectures*, *OnZientzia*, *top@DIPC*, *nanoKOMIK*, *Mestizajes*, and the popular *Passion for Knowledge* festivals, among others.

All in all, we at DIPC believe that a world without science would be a much worse place to live.

But we also believe that science isolated from society would lose a substantial part of its relevance. Hence, we are as much committed to the generation of new knowledge as to sharing the joy of these discoveries with the world. ■

Pedro Miguel Echenique
President

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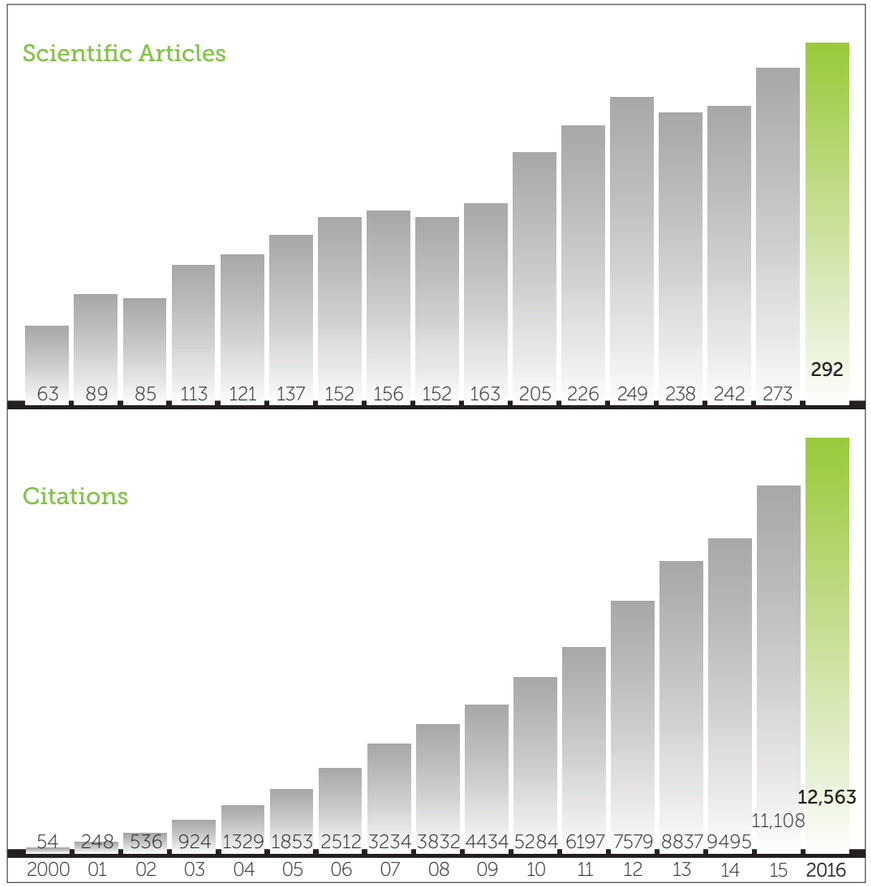
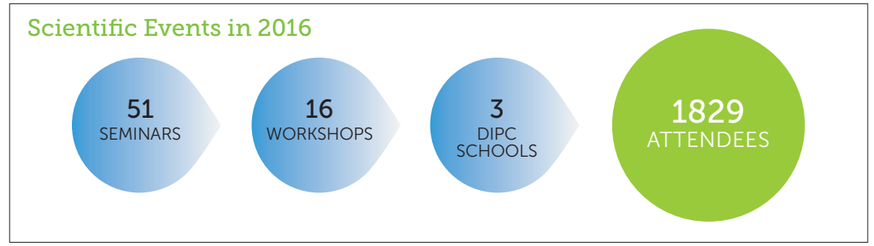
Research Activity at a Glance

DIPC's scientific production and international impact continues to increase. Since its creation, during the last 17 years, the center has published a total number of **3,050 ISI publications** and has received more than **83,413 citations**. The **292 scientific articles** and **four book chapters** published in 2016 mean an increase of **468%** in the number of publications as compared to 2000.



Source Web of Science Core Collection (all years & indexes) - DIPC's ResearcherID C-3171-2014 (02/05/2017)



In addition to doing research, DIPC's annual strategic agenda of actions foster exchange with scientists from around the world. Included in the program are Seminars by international experts which cover particular research topics, Workshops on specific subjects of interest, and the DIPC Schools which focus on learning particular skills.

Driving Force of DIPC's Research Activity: Our Highly Dynamic Community

In addition to PhD students and postdoctoral researchers, who come from other institutions to complete their training and expertise, the core of the DIPC Community is made up of local scientists. Some of them are spread over other centers in different faculties of the University of the Basque Country and the Materials Physics Center and are distinguished such as the DIPC Associates. The local scientists act as hosts for the large number of international visiting researchers and retain the scientific-technical knowledge in the local environment developing long term DIPC research projects. Among the local host community, there are also Ikerbasque Researchers and Gipuzkoa Fellows, the latter being DIPC's star program in regard to attracting, retaining, and looking after scientific talent.

DIPC Supercomputing Center

The Supercomputing Center at DIPC is its great strategic infrastructure and serves as a fundamental tool for the excellent research carried out by our researchers

Computational physics and chemistry are among the strongest research fields in the Basque Country and the Supercomputing Center is one of its key resources. With its current level of physical, human and technical resources this high performance computing (HPC) center has become a focus of technological knowledge, training, and innovation. Its status and influence transcend its primary mission, not only as a tool but also as a discipline in itself. There is no more powerful computing center of its type in the Basque Country.

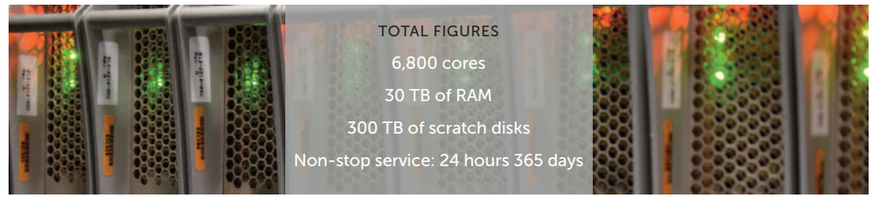
"The variety and power of the computing resources of DIPC, and its constant upgrade, allow the permanent confrontation of a wide range of numerical simulations that put DIPC at the forefront in research."

Txomin Romero Asturiano
Director of the Supercomputing Center

Current computing resources

The Center has three rooms to host the HPC systems. These rooms have an isolated electrical connection, communications infrastructure, humidity, electricity consumption and temperature control sensors, various uninterrupted power supply systems, refrigeration systems, automatic fire-extinguishing systems and intrusion detection.

As of 2016, the Center has **six different supercomputers covering a wide range** of computational needs, from Xeon E5-2680 V3 nodes with 24 cores, 256 GB of RAM and Infiniband FDR connection, large shared memory computers with 1024 cores and 4 TB of RAM in a single operating system image, to nodes with NVIDIA Geforce GPU technology for GPGPU programming or Xeon Phi technology.



More than 140 researchers from DIPC and other research centers such as the UPV/EHU, the CSIC-UPV/EHU Materials Physics Center, CIC nanoGUNE or Ikerbasque used this computational infrastructure in 2016.

The European Physical Society has awarded DIPC a distinction

in recognition of its

outstanding contributions in the fields of

condensed matter physics and materials science,

as well as for its successful

outreach activities

This distinction for science outreach was the first in a series that shall be awarded by EPS to European institutions or individual researchers in recognition of their work in the promotion and fostering of a scientific culture.

Members of the DIPC Board of Trustees during the uncovering of the distinctive plaque on the wall of the center, next to the main entrance (15/12/2016). From left to right: Alberto López Basaguren, Juan Colmenero, Ricardo Díez Muiño, Ainhoa Aizpuru Murua and Pedro Miguel Echenique (center) showing the EPS award plaque, Amaia Esquisabel Alegría, Carlos Ruiz, Adolfo Moráis, Andres Arizkorreta, Leire Bilbao.

"It is fantastic to have the opportunity to recognize the achievements of a center such as DIPC, which for 16 years, has been striving for excellence in science and also in communication."

"It is important to acknowledge the effort made by the President of DIPC, Pedro Miguel Echenique, and also its Director, Ricardo Diez Muiño, in developing DIPC, here in San Sebastian.
DIPC has devoted a long time to promoting and catalyzing high-level research in condensed matter physics and materials science.
The center is a platform on which ideas are freshly exchanged and new objectives are continuously set and shared.
It is at the cutting edge of science; publishing many papers in well recognized journals. It assumes a primary role in the responsibility of conveying scientific knowledge to society, and is firmly convinced, as we are at EPS, that scientific culture contributes to the progress and freedom of society."

Christophe Rossel
President of the European Physical Society

The plaque was presented by the president of the EPS, Christophe Rossel (left with Pedro Miguel Echenique, and right with Cristina Uriarte and Ricardo Diez Muiño) on the closing day of Passion for Knowledge 2016. On September 30th and October 1st DIPC also hosted the annual EPS Executive Committee's meeting at its headquarters in San Sebastián.

Science Communication

Promoting science as a key cultural activity

The extensive science communication program at DIPC helps to establish a fluid and permanent dialogue between science and society.

The amount, variety, and impact of DIPC's outreach activities are continuously increasing, with a participation of more than **13,300 people** during 2016.

Eneko Goya, Pedro Miguel Echenique, Lehendakari of the Basque Government Iñigo Urkullu (center), Markel Olano, and Cristina Uriarte just before the opening ceremony of Passion for Knowledge 2016 on September 27th.

PASSION FOR KNOWLEDGE

Much more than a science festival

The science festivals hosted by DIPC have already become an anticipated engagement for all citizens interested in recent advances in different disciplines of knowledge.

In 2016, from September 27 to October 1, the third and latest event in the series of Passion for Knowledge festivals was celebrated. Integrated into the program of the **European Capital of Culture** held by the city of San Sebastian in 2016, the occasion served to highlight science as an essential part of culture. Full of different activities for both adult and young audiences, Passion for Knowledge 2016 attracted more than 9,600 spectators.

Victoria Eugenia Theatre in San Sebastian, main venue of Passion for Knowledge 2016.

The Public Lectures of Passion for Knowledge 2016, attended by close to 3,000 people, were once again at the core of this festival of science, knowledge, culture and passion. The highlight of these sessions were the Plenary Lectures delivered by 13 prestigious speakers from different scientific disciplines, including four Nobel laureates that combined scientific rigour with entertainment to awaken curiosity, interest, enthusiasm and critical thinking of society.








27 SEPTEMBER – 1 OCTOBER **2016**

Plenary Lectures

Dudley Herschbach Physical-Chemistry, Harvard University, USA
The Impossible Takes a Little Longer

Andrew Blake Software Engineering, The Alan Turing Institute, UK
Machines that learn to see

Dame Jocelyn Bell Burnell Astrophysics, Oxford University, UK
Cosmic Fireworks: finding transient events in the Universe

Sir John Pendry Photonics, Imperial College London, UK
Metamaterials open new horizons in electromagnetism

William Friedman Botany, Harvard University, USA
Tales of Obsession in a Botanical Garden of Trees

Álvaro de Rújula Physics, CERN, Switzerland; Instituto de Física Teórica UAM-CSIC, Spain
La creación en las artes, en las ciencias y en los mitos (el bosón de Higgs y todo lo demás)

Agustín Sánchez-Lavega Planetary Atmospheres, University of the Basque Country, Spain
Planetas en otras estrellas

Elena Cattaneo Biology, Università degli Studi di Milano, Italy
Stories of Science, cells and freedom

Martin Karplus Chemistry, Harvard University, USA; Université de Strasbourg, France
Motion: Hallmark of Life. From Marsupials to Molecules

Rafael Yuste Neurobiology, Columbia University, USA
Las Nuevas Neurotecnologías; Implicaciones para la Ciencia, Medicina y Sociedad

Claude Cohen-Tannoudji Physics, École Normale Supérieure, France
Science as an integral part of the culture

Alessandra Buonanno Physics, Max Planck Institute for Gravitational Physics, Germany
Sounds of Silence: Listening to the Universe with Gravitational Waves

Klaus von Klitzing Physics, Max Planck Institute for Solid State Research, Germany
A New Kilogram in 2018: The Biggest Revolution in Metrology since the French Revolution

http://**p4k.dipc**.org

ROUND TABLE on Creativity

29/09/2016

Moderated by the President of DIPC and Chairman of Passion for Knowledge, **Pedro Miguel Echenique**, the Round Table featured four renowned specialists from different branches of the Humanities, who talked about the intangible yet so valuable thing that is creativity, on the basis of their individual expertise and knowledge.

Itziar Laka Linguist, UPV/EHU
Kirmen Uribe Writer, Basque Country
Juan Ignacio Pérez Physiologist, UPV/EHU
Rafael Yuste Neurobiologist, Columbia University, USA

BERTSOLARIAK

30/09/2016

Knowledge is not the exclusive domain of either the Arts or Science, that is why Passion for Knowledge did not only focus on science. There was room for all branches of knowledge, including one that exclusively belongs to the Basque culture: the art of Basque improvised sung poetry.

Amets Arzallus
Andoni Egaña
Maialen Lujanbio

Three of the Basque Country's most talented and well-known versifiers or improvisational poets, locally called "bertsolaris" gave a masterclass on the different ways of composing a 'bertso' or sung poem, and provided some insight into the creative process underlying this improvised art.

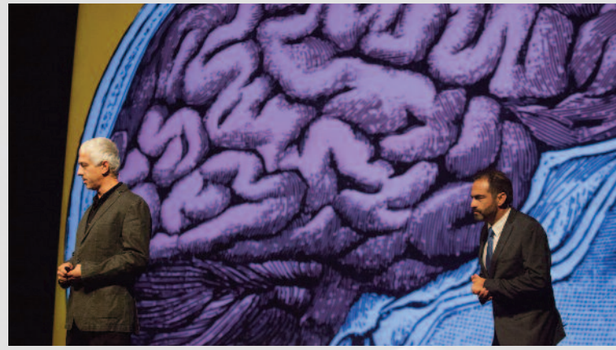
BREAKING BOUNDARIES Convergence, Collaboration and Integration

27/09/2016

Breaking Boundaries is an innovative and immersive live art installation combining sculpture, dance, video and sound which was created by UK based artists **Melissa Pierce Murray** and **Diana Scarborough** for the inauguration of Passion for Knowledge 2016. The artists used scientific concepts such as mind mapping or particle/wave duality to generate the choreography, and worked with local dancers from the dance company **Dantzaz**, to create a unique evocative performance piece.

This project was produced by DIPC in collaboration with Dantzagunea.

NAUKAS PASSION



Coordinated by the *Chair in Scientific Culture of the UPV/EHU*, the talks by the popular online platform for scientific communication and dissemination, *Naukas, science, scepticism and humor,* were another essential part of the festival's program.

28/09 and 30/09/2016

Following the plenary lectures, 12 of Naukas' best collaborators went up on stage to offer the public their own somewhat quirky take on different scientific subjects in a series of simple, dynamic, amusing and original 10-minute talks.

01/10/2016

Código Sapiens
Xurxo Mariño Neuroscientist and science populariser, University of A Coruña
Vicente Mohedano Actor

The cherry on the cake of the section was a 'Discurshow' or theatralised talk about the language and the mysteries that surround its appearance in the evolutionary process.

LA COULEUR DES ANNÉES CINQUANTE Photography exhibition

During the fifties and sixties, American chemist **Martin Karplus**, Nobel Laureate in Chemistry 2013, travelled extensively throughout the world with his Leica camera and made thousands of color photographs on early Kodachrome slide film. The exhibition 'Colour of the 50s', comprised of about a hundred of these images, was first shown at the Bibliothèque Nationale de France and; after being exhibited in various cities around the world, the collection remained on display in the Aquarium of San Sebastián from September 26th to November 20th, 2016.

ZIENTZIA KLUBA

01/10/2016

This session was specially aimed at the youngest public and their families and gathered together over 120 people in the Club Room of the Victoria Eugenia Theatre. The mini science festival was carried out in Basque and featured amusing and funny scientific activities, including live experiments, scientific storytelling and monologues:

SCIENTIFIC STORYTELLING

Ana Galarraga Elhuyar
Marikalanbre bizitzaren laborategian

PRESENTATIONS AND EXPERIMENTS

Aitor Bergara UPV/EHU, DIPC
Lebitazioa, magia eta are gehiago

Koldo García UPV/EHU
Geneetan daramagun superheroia

Eider San Sebastián UPV/EHU
Material berri "harrigarriak" kimikaren ikuspuntutik

Jon Mattin Matxain UPV/EHU, DIPC
Suaren koloreak

PhD Training

Science dissemination in society is becoming increasingly important, and in this vital task all members of the scientific community have a role to play, including doctoral or PhD students. Within the framework of the festival Passion for Knowledge 2016, a group of 15 students from the European Excellence Innovative Training Network ITN-EJD-TCCM (European Joint Doctorate in Theoretical Chemistry and Computational Modelling) organized, participated in and promoted a series of outreach training activities.

The activities were a series of three interconnected and complementary events:

MEET THE PROFESSOR

Informal meetings with Nobel Laureates.
DIPC, Donostia / San Sebastian

27/09/2016
Martin Karplus

29/09/2016
Dudley Herschbach

ENCOUNTER WITH SECONDARY SCHOOL STUDENTS

Face to face chats with students.
28/09/2016
La Salle Institute, Donostia / San Sebastian

DIVULGATION PAPERS FOR A BLOG

Popular science articles for the blog
Mapping Ignorance: http://mappingignorance.org
October-December 2016

PASSION FOR KNOWLEDGE Committee

Chairman of Passion for Knowledge 2016
Pedro Miguel Echenique President of DIPC and Professor at the UPV/EHU

General Coordinator
Nora Gonzalez Outreach Manager of DIPC

Ricardo Díez Muiño Director of DIPC
Igor Campillo Executive Director of Euskampus
Juan Ignacio Pérez Coordinator of the Chair in Scientific Culture at the UPV/EHU
Amaia Arregi Outreach Officer at DIPC
Xabier López Lecturer at the UPV/EHU
Itziar Otegui Outreach Manager of CIC nanoGUNE
Jon Mattin Matxain Researcher from the UPV/EHU

top@DIPC Encounters. Zientziarekin solasean!

DIPC organized the 8th edition of the annual Encounters between Nobel Laureates and leading researchers with high schools students. This time the encounters *top@DIPC - Zientziarekin solasean!* were held in the framework of the festival Passion for Knowledge 2016.

The main aim of these informal encounters is to foster students' interest in scientific and technological studies. To achieve so, prestigious guest scientists talk about their passion for science and research and answer questions asked by the participant students about their lives and experiences throughout their professional careers. This edition included two encounters:

28/09/2016
Bizkaia Aretoa UPV/EHU, Bilbao

Martin Karplus
Harvard University, USA;
Université de Strasbourg, France
Nobel Laureate in Chemistry 2013

Dame Jocelyn Bell Burnell
Oxford University, UK

Claude Cohen-Tannoudji
École Normale Supérieure, France
Nobel Laureate in Physics 1997

Hosts: **Cristina Uriarte**, Regional Minister for Education, Language Policy and Culture, Basque Government; **Iñaki Goirizelaia**, Rector of the University of the Basque Country; **Javier Benito**, Director of Telefónica Euskadi

30/09/2016
Eureka! Science Museum, Donostia / San Sebastian

Elena Cattaneo
Università degli Studi di Milano, Italy

Dudley Herschbach
Harvard University, USA
Nobel Laureate in Chemistry 1986

Pamela Diggle
University of Connecticut, USA

Hosts: **Adolfo Morais**, Deputy Regional Minister for Universities and Research, Basque Government; **Rafael Careaga**, Head of Resources and Institutional Relations, EDP naturgas energia; **Ignacio Zuzuarregui**, Director, Eureka! Zientzia Museoa

Telefónica and **EDP naturgas energia**, long time patrons of DIPC, participated and sponsored the encounters held in Bilbao and San Sebastian respectively, by giving an award to the most ingenious, interesting or original questions sent by the participating students.

A total of **87 schools** from all over the Basque Country participated in the encounters, which were attended by **476 students** and **99 teachers**.

Kutxa Lectures

The Kutxa Lectures, organized in collaboration with Kutxa Obra Social in San Sebastian, started in 2010. Speakers include renowned scientists and Nobel laureates as well as science communicators and humanists working in the frontiers of science.

29/02/2016
Kutxa Andia Hall
El primer descubrimiento Advanced LIGO. Las ondas gravitacionales detectadas 100 años después de la predicción de Einstein

Alicia M. Sintes Olives and **Sascha Husa**
University of the Balearic Islands (UIB), Spain

For the first time, scientists have detected gravitational waves: ripples in the fabric of space-time which travel to Earth from big catastrophic events occurring in the Universe. This discovery fulfills the last prediction of Einstein's general theory of relativity proposed in 1915, opening a new window in the observation of the Universe. First gravitational waves were detected the 14th September 2015 by the twin detectors from the Laser Interferometer Gravitational-Wave Observatory (LIGO) in the USA.

High School Visits

In 2016, DIPC together with the Material Physics Center (CFM) continued the program of visits for groups of high school students launched in 2014. Both centers open their doors so these young students can meet researchers and view their work close up. **During 2016 DIPC and CFM hosted a total of 362 students from 14 schools.**

On Zientzia

26/05/2016

The award ceremony of the sixth edition of the On Zientzia video contest organized jointly by DIPC and Elhuyar Foundation took place at the headquarters of Donostia / San Sebastián 2016 European Capital of Culture. It was later broadcasted on the TV program *Teknopolis*. The awardees were:

YOUNG PRIZE
El mecanismo de la vida
Leonel Virosta (Student, 17 years old, Cantabria)

BEST VIDEO IN BASQUE
Teleskopioak
Mikel Ramírez (Audiovisual professional, Basque Country)

BEST VIDEO
Soy esa bacteria que vive en tu intestino
Julio Ruiz (Teacher, Slovakia)

SPECIAL MENTIONS
El mito de Arquímedes
Eneko Amezaga (Basque Country)
Asiar Liztorra
Students of 1st grade of Compulsory Secondary Education, IES Elorrio (Basque Country)
Several videos
Guillermo Ordás (17 years old, Basque Country)

In this sixth edition of On Zientzia, 53 videos participated, among them 26 within the Young Prize category, and 19 videos were in Euskera. Altogether the website of the contest contains a repository of more than 270 videos.

19/10/2016
The seventh edition of On Zientzia was launched which included the release of a brand new image for the website.

For more information visit:
www.onzientzia.tv

Science Week

PhD students, young post-doctoral researchers and communicators from DIPC, Materials Physics Center (CSIC-UPV/EHU) and CIC nanoGUNE participated together with a stand called *Exploring the tiny world* at the Science Week organized by the University of the Basque Country.

03-05/11/2016
Kursaal Congress Center
Donostia / San Sebastián

nanoKOMIK

DIPC and CIC nanoGUNE launched the nanoKOMIK project in 2016 for the **creation of the first participative nanofiction comic**. This is a science outreach initiative of a participatory, multidisciplinary, and international nature that seeks to make society aware of the advances that are being made in the field of nanoscience and nanotechnology, in this way awakening the creativity of the younger generation. The project was created and coordinated by Amaia Arregi (DIPC) and Itziar Otegui (CIC nanoGUNE).

nanoKOMIK challenge
In the first stage of the project, the challenge involved more than 150 young people aged between 12 and 18 in a free creative process where they created their female and male comic superheroes, providing them with nanopowers through astonishing features acquired by matter thanks to nanoscience and nanotechnology.

Over 100 youngsters participated in the **science and comic workshops** held in different towns during January to April:
30/01/2016 Bilbao, Paraninfo UPV/EHU
06/02/2016 Donostia / San Sebastián, FNAC
20/02/2016 Vitoria-Gasteiz, Artium
27/02/2016 Iruñea/Pamplona, Palacio Condestable
16/03/2016 Donostia / San Sebastián, CIC nanoGUNE
18/03/2016 Iruñea/Pamplona, Mendillorri High School
13/04/2016 Bayonne, Médiathèque

Moreover, a special session intended for science and art high school teachers took place at CIC nanoGUNE. The workshops were guided by scientists Jon Ander Arregi, Amaia Arregi and cartoonists Jose Carlos Torre, and Marko (Le Godillots).

Publication of the collective nanofiction comic
In the second phase, based on the best ideas from the comics presented in response to the challenge, the collaborative comic *Dayanne and Murillo. The power of nanoscience* was elaborated hand in hand with the professional cartoonist Hodei Iparraguirre.

The book was presented in the opening of its itinerant exhibition, and then, distributed to all public libraries of the Basque Country and participants. It is also available on www.nanokomik.com.

Award Ceremony

10/06/2016
Headquarters of
Donostia / San Sebastián
2016 European Capital of Culture
(DSS2016)

At the prize giving ceremony, a collective exhibition containing the more than a hundred works presented in the challenge was inaugurated. Ricardo Díez-Muiño, director of DIPC, Txema Pitarke, director of CIC nanoGUNE, Sonia Arnés, representative of FECYT, and Lorena Montejo, head of the *Faro de las Voces* of DSS2016, participated in the prize-giving. The three main awards were submitted by a formal jury, together with the audience award:

FIRST PRIZE
Crisis cardiaca
Dayanne Huayhua Calicho, Aranjuez

SECOND PRIZE
Milan Man
Asier Murillo Iriarte, Iruñea / Pamplona

SPECIAL MENTION
Lizard Guy – El hombre lagarto
Elena Vergel Pla, Lleida

AUDIENCE AWARD
Hielo y Fuego
Claudia Araujo Vallejo, Castro Urdiales

After the prize-giving, the attendees enjoyed a scientific, humorous show specially created for nanoKOMIK: "NANO".
Albert Vivó, The Big Van's monologuist

For more information visit:
www.nanokomik.com

02-30/12/16
Itinerant exhibition
Dayanne eta Murillo. Nanozientziaren indarra.
Carlos Santamaría Center UPV/EHU,
Donostia / San Sebastián

Mestizajes

Mestizajes is a trans-disciplinary program coordinated by **Gustavo Ariel Schwartz** that bridges the gap between artistic, social and scientific branches of the humanities. Through a series of workshops, lectures, visits and collaborations, Mestizajes encourages people to take a critical look at reality from an innovative cutting-edge perspective.

SEMINARS

17/05/2016
Sala de Actividades de la Biblioteca Central, Donostia / San Sebastián
"De asesinatos, detectives y teoremas - Matemáticas en la novela negra"
Raúl Ibánez Torres, UPV/EHU

25/05/2016
DIPC, Donostia / San Sebastián
"Quantum Poetics: Language and Reality in Physics and Poetry"
Amy Catanzano, writer and poet, USA
This visit to DIPC was part of a research experiment about quantum poetics that led Catanzano also to CERN.

07/06/2016
DIPC, Donostia / San Sebastián
"Cultural Analytics.
The Humanistic Science of Culture."
Juan Luis Suárez, CulturePlex Lab in Western University (Ontario), Canada

Presentation of the book "The interview"

"The interview" is a theatre play co-written by **Luisa Etxenike** and **Gustavo Ariel Schwartz** which was performed with great success in different towns of our geography in 2013. In 2016, the publication of the play in a bilingual edition (Spanish/English) by the publisher El Gallo de Oro was presented in Donostia / San Sebastián, Bilbao and Madrid.

Realidad Conexa

Connected Reality is an audiovisual project in which the links and connections between different spheres of knowledge are presented with an original, modern and highly meticulous aesthetic approach. In particular, what it shows are the relations between science, art and literature. The project was coordinated by **Gustavo Ariel Schwartz** and **Ana Montserrat**, and was presented at Passion for Knowledge 2016.

The eight capsules of *Connected Reality* are available in Spanish and English in https://vimeo.com/-channels/mestizajes, where they had more than 11,500 views in the first six months.

For more information visit:
www.**mestizajes**.com

Urbanzientzia

21/05/2016
Urbanzientzia was an activity proposed within **Olatu Talka**, an annual popular festival which was launched in 2010 within the framework of the Capital of Culture of Donostia / San Sebastián. Its goal is driving and fostering citizen initiatives in the street and in 2016 DIPC participated together with CFM and CIC nanoGUNE with a stand about nanoscience.

DIPC Events in Neighboring Cities:
Bilbao, Vitoria-Gasteiz, Pamplona, Bayonne and Bordeaux

nanoKOMIK - Science and Comic Workshops
Bilbao (Paraninfo UPV/EHU), Vitoria-Gasteiz (Artium), Iruñea/Pamplona (Condestable Palace and Mendillorri High School) and Bayonne (Médiathèque)
Guided by **Jon Ander Arregi** and **Jose Carlos Torre**, and in Bayonne by **Amaia Arregi** and **Marko**

Events organized within Passion for Knowledge 2016

28/09/2016
Bizkaia Aretoa UPV/EHU, Bilbao
Public lecture by **Klaus von Klitzing**, Nobel Laureate in Physics 1985

28/09/2016
Bizkaia Aretoa UPV/EHU, Bilbao
Encounters with high school students with:
Martin Karplus, Nobel Laureate in Chemistry 2013
Dame Jocelyn Bell Burnell
Claude Cohen-Tannoudji, Nobel Laureate in Physics 1997

29/09/2016
Amphithéâtre Pitres, Université de Bordeaux, France
Public Lecture by **Sir John Pendry**

DIPC 2016 The Year in Media

177	418	17+	80+
newspaper articles	news online	television appearances	radio mentions

Scientific Highlights

Single-molecule optomechanics in 'pico-cavities'

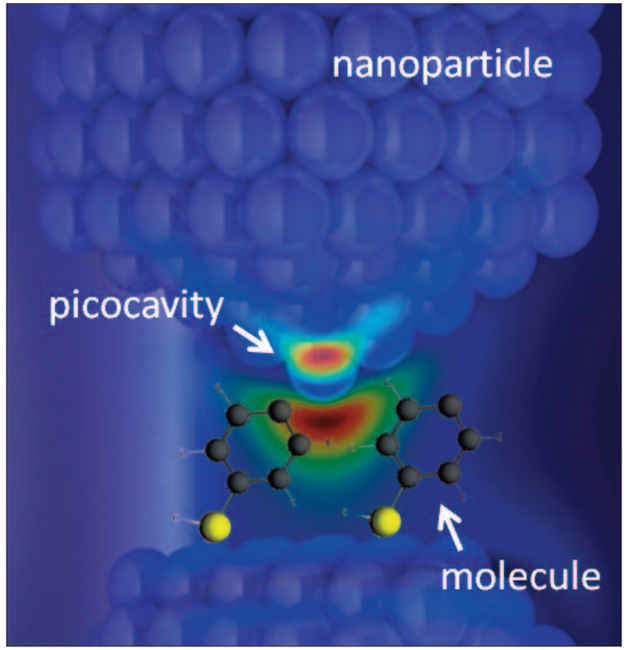
F. Benz, M.K. Schmidt, A. Dreismann, R. Chikkaraddy, Y. Zhang, A. Demetriadou, C. Carnegie, H. Ohadi, B. de Nijs, R. Esteban, J. Aizpurua, and J.J. Baumberg
Science 354, 725-729 (2016)

The diffraction limit states that light cannot be focused by conventional systems to arbitrarily small regions, the minimum size being limited to about half the wavelength of light, corresponding to a few hundred nanometers for visible light in vacuum or in a dielectric. However, the excitation of surface plasmons —collective oscillations of the free electrons of metals— allows strongly enhancing the optical energy in an extremely small 'hot-spot' region. Picocavities push light-focusing to the subnanometer region, which introduces the possibility to manipulate individual vibrations of a molecule.

Plasmon resonances are exploited in a variety of spectroscopy techniques that serve to characterize molecules. In Raman Spectroscopy, for example, differences of energy between incoming and outgoing photons provide a fingerprint of the vibrations of the molecule. Standard Raman is very little efficient, but in Surface-Enhanced Raman Spectroscopy (SERS) the strong confinement of the plasmonic field leads to a very large enhancement of the coupling strength between light and the molecule, allowing to detect the signal emitted by even a single molecule. Picocavities squeeze hot spots to the dimensions of molecules thus making them useful not only to study and spatially resolve single molecules in dense samples, but also to reveal novel phenomena that emerge as the coupling strength is pushed to its limit.

Researchers at the DIPC and Centro de Física de Materiales (CSIC-UPV/EHU) in San Sebastián and the University of Cambridge have reported in *Science* that they are able to control the optical response of picocavities by harnessing the natural wandering of atoms in gold particles. The authors first use a molecular layer to create a nanometer gap between a plasmonic particle and a metallic substrate. In such a structure, an atom will occasionally protrude from the surface, creating the plasmonic picocavity, which can be detected by carefully monitoring the activity of the Raman signal of the molecules in the gap. By keeping the temperature at cryogenic temperature, the movement of atoms can be made weak enough for the picocavity to be stable.

The research team compares the SERS measurements with predictions from model atomistic calcualtions and show that the subnanometer confinement of light –with the corresponding strong gradient– makes it possible to efficiently interact with molecular vibrations that would not be excited in a conventional Raman experiment. Remarkably, different picocavities allow for selective excitation of individual vibrations



Illustrative image of the molecule-plasmon interaction in a picocavity. The region between an atomic-scale feature in a plasmonic nanoparticle and a metallic substrate (another nanoparticle or a flat surface) constitutes a picocavity, which is characterized by optical fields spatially confined to the subnanometer scale. When a molecule is placed in the picocavity, the light can interact strongly with molecular vibrations via Surface Enhanced Raman. The obtained signal can be seen as the consequence of molecular optomechanical processes.

Different picocavities allow for selective excitation of individual vibrations of the molecule

of the molecules. Last, the researchers use a recently developed theoretical framework that treats SERS in analogy to optomechanical systems. This optomechanical analysis reveals that the plasmon-vibration coupling strength characterizing the picocavity system is extremely large, indicating that these molecular optomechanical systems can approach the single-photon strong-coupling limit, a regime of large interest for the study of quantum phenomena.

Beyond Dirac and Weyl fermions: unconventional quasiparticles in conventional crystals

B. Bradlyn, J. Cano, Z. Wang, M.G. Vergniory, C. Felser, R.J. Cava, and B.A. Bernevig
Science 353, aaf5037 (2016)

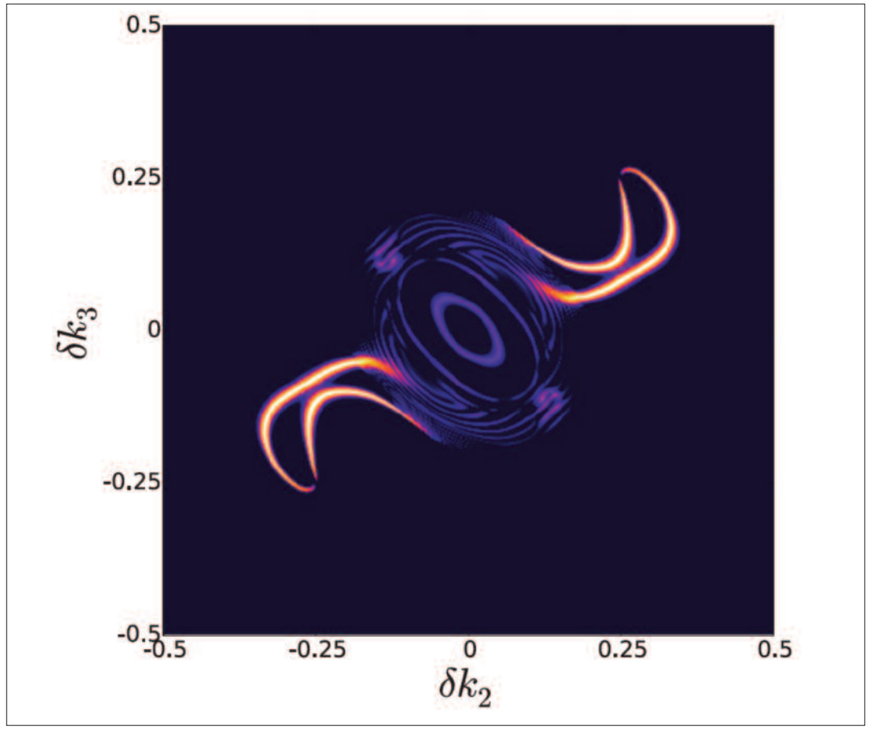
An international team of researchers has predicted the existence of several previously unknown types of quantum particles in materials. The particles — which belong to the class of particles known as fermions — can be distinguished by several intrinsic properties, such as their responses to applied magnetic and electric fields. In several cases, fermions in the interior of the material show their presence on the surface via the appearance of electron states called Fermi arcs, which link the different types of fermion states in the material's bulk.

The research, published in the journal *Science*, was conducted by a team at Princeton University in collaboration with researchers at the Donostia International Physics Center (DIPC) in Spain and the Max Planck Institute for Chemical Physics of Solids in Germany. The investigators propose that many of the materials hosting the new types of fermions are "protected metals" which are metals that do not allow, in most circumstances, an insulating state to develop. This research represents the newest avenue in the physics of "topological materials" an area of science that has already fundamentally changed the way researchers see and interpret the states of matter.

The team at Princeton included Barry Bradlyn and Jennifer Cano, both associate research scholars at the Princeton Center for Theoretical Science; Zhijun Wang, a postdoctoral research associate in the Department of Physics, Robert Cava, the Russell Wellman Moore Professor of Chemistry; and B. Andrei Bernevig, associate professor of physics. The research team also included Maia G. Vergniory, a Fellows Gipuzkoa researcher at DIPC, and Claudia Felser, a professor of physics and chemistry and director of the Max Planck Institute for Chemical Physics of Solids.

For the past century, gapless fermions, which are quantum particles with no energy gap between their highest filled and lowest unfilled states, were thought to come in three varieties: Dirac, Majorana and Weyl. Condensed matter physics, which pioneers the study of quantum phases of matter, has become fertile ground for the discovery of these fermions in different materials through experiments conducted in crystals. These experiments enable researchers to explore exotic particles using relatively inexpensive laboratory equipment rather than large particle accelerators.

In the past four years, all three varieties of fermions have been theoretically predicted and experimentally observed in different types of crystalline materials grown in laboratories around the world. The Weyl fermion was thought to be last of the group of predicted quasiparticles in nature. Research published earlier this year in the journal *Nature* (Wang et al., doi:10.1038/nature17410) has shown, however, that this is not the case, with the discovery of a bulk insulator which hosts an exotic surface fermion.



Two electronic states known as Fermi arcs, localized on the surface of a material, stem out of the projection of a 3-fold degenerate bulk new fermion. This new fermion is a cousin of the Weyl fermion discovered last year in another class of topological semimetals. The new fermion has a spin-1, a reflection of the 3- fold degeneracy, unlike the spin-½ that the recently discovered Weyl fermions have.

In the current paper, the team predicted and classified the possible exotic fermions that can appear in the *bulk* of materials. The energy of these fermions can be characterized as a function of their momentum into so-called energy bands, or branches. Unlike the Weyl and Dirac fermions, which, roughly speaking, exhibit an energy spectrum with 2- and 4-fold branches of allowed energy states, the new fermions can exhibit 3-, 6- and 8-fold branches. The 3-, 6-, or 8-fold branches meet up at points – called degeneracy points – in the Brillouin zone, which is the parameter space where the fermion momentum takes its values.

During the search for materials exhibiting the new fermions, the team uncovered a fundamentally new and systematic way of finding metals in nature. Until now, searching for metals involved performing detailed calculations of the electronic states of matter. The researchers suggest that this is because the new fermions require multiple electronic states to meet in energy: The 8- branch fermion requires the presence of 8 electronic states. As such, a system with only 4 electrons can only occupy half of those states and cannot be insulating, thereby creating a protected metal.

Fully fused quinoidal/aromatic carbazole macrocycles with poly-radical characters

S. Das, T.S. Herng, J.L. Zafra, P.M. Burrezo, M. Kitano, M. Ishida, T.Y. Gopalakrishna, P. Hu, A. Osuka, J. Casado, J. Ding, D. Casanova, and J. Wu
Journal of the American Chemical Society 138, 7782-7790 (2016)

This work represents the first demonstration of singlet π-conjugated molecules with poly-radical characters.

π-Conjugated molecules with open-shell singlet ground state have drawn immense attention of researchers worldwide due to their unique optical, electronic and magnetic properties that make them attractive for non-linear optical materials, field effect transistors, and organic spintronics. Successful isolation of various relatively stable diradicaloids motivates us to work towards molecules with poly-radical character. Theoretically, graphene nanoribbons (including long acenes) with elongated zig-zag edges may develop diradical and even poly-radical character in the electronic ground state. This behavior has been experimentally validated in small size polycyclic aromatic hydrocarbons (PAHs) such as teranthene and quarteranthene, which show moderate to large diradical character. However, synthesis and isolation of PAHs beyond diradicals, i.e. with higher radical character in the singlet ground state, remains as a challenging task due to tedious synthesis and their intrinsic instability.

The difficulty in modeling organic molecules possessing poly-radical characters can be mainly ascribed to the strong anti-ferromagnetic bonding interactions between the multiple spins in the singlet ground-state. In other words, the presence of strong polyradicaloid nature in singlet ground state molecules requires sufficient driving force from closed-shell form to open-shell diradical form and then to higher poly-radical forms. Previous studies have demonstrated that recovery of one or more aromatic sextet rings in the diradical form was one of the major driving forces to obtain molecules with a significant diradical character. In this study, we report the design, challenging synthesis and physical characterization of two fully-fused carbazole macrocycles 4MC and 6MC, which contain four and six alternatingly arranged quinoidal and aromatic carbazole units, respectively (Figure 1). The quinoidal carbazole moiety is fundamentally an analogue of pro-aromatic Tschitschibabin's hydrocarbon and has an irresistible tendency to recover two aromatic sextet rings in the diradical form. Such a simple analysis can be applied to 4MC and 6MC, in which two aromatic sextets are gained at each stage of transition from closed-shell form to open-shell diradical form, and then to tetraradical form and finally to hexaradical form (Figure 1).

Various experimental measurements and advanced theoretical calculations indicate that the two fully fused quinoidal/aromatic carbazole macrocycles, 4MC and 6MC compounds, display very high poly-radical characters in the singlet ground state. They can be regarded as the first true open-shell organic singlet tetraradicaloid and hexaradicaloid molecules, respectively (Figure 2). Both compounds have small excitation energy gaps and can be thermally populated to high spin excited states, which results in interesting magnetization behavior even at room temperature. Although the magnetization is very weak, it may imply an alternative approach to design molecular magnets in the future. Assuming that one can synthesize 2D and 3D rigid organic frameworks with poly-radical characters in a singlet ground state, thermal population to high spin states could become significant and the long arrange ordered alignment of the spin would eventually lead to significant magnetization at higher temperature.

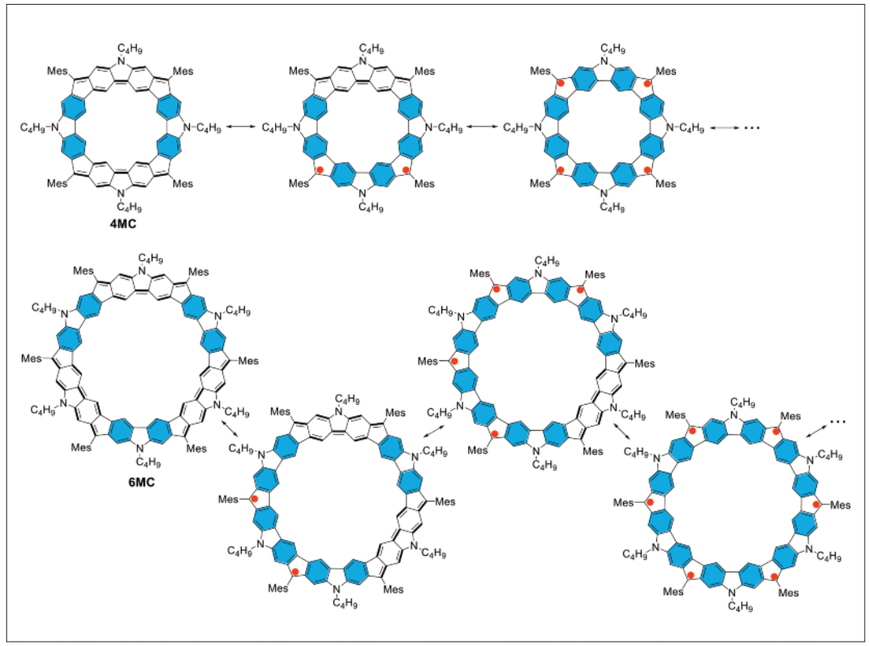


Figure 1. Closed-shell and open-shell canonical forms of 4MC and 6MC. Clar's aromatic sextets are highlighted in blue hexagon.

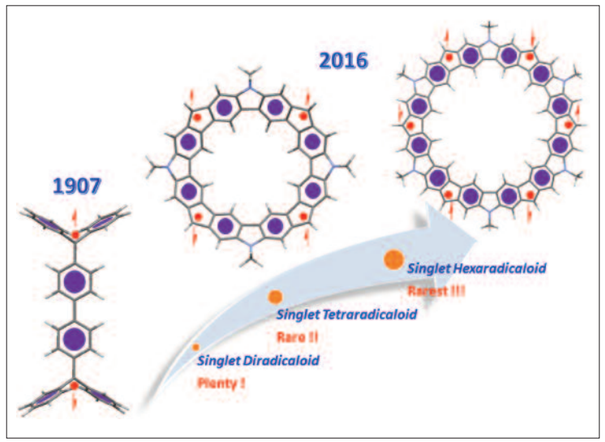


Figure 2.
First true open-shell organic singlet tetraradicaloid and hexaradicaloid molecules.

An alternative approach to design molecular magnets in the future

Quantum hydrogen-bond symmetrization in the superconducting hydrogen sulfide system

I. Errea, M. Calandra, C.J. Pickard, J.R. Nelson, R.J. Needs, Y. Li, H. Liu, Y. Zhang, Y. Ma, and F. Mauri
Nature 532, 81-84 (2016)

The quantum behavior of hydrogen affects the structural properties of hydrogen-rich compounds, possible candidates for room-temperature superconductivity. Hydrogen is the atom more strongly subjected to quantum behavior. New theoretical results suggest that its quantum nature strongly affects the recently discovered sulfur hydride superconductor, a compound that at high pressure has the highest critical temperature reported for any superconductor. This new step towards understanding the underlying physics of high temperature superconductivity was published in *Nature*.

What governs the behavior of objects in our daily life is a classical deterministic physics, that is, Newton's laws. These daily objects have both a determined position and velocity. This means, for example, that we can track an object over time. However, this is not possible in the atomic world, the quantum world. According to Heisenberg's uncertainty principle, the velocity and position of a particle cannot be determined at the same time. As a consequence, instead of having a specific position, particles appear to us as described by a broad wave function that tells us only where it is more probable to find the particle.

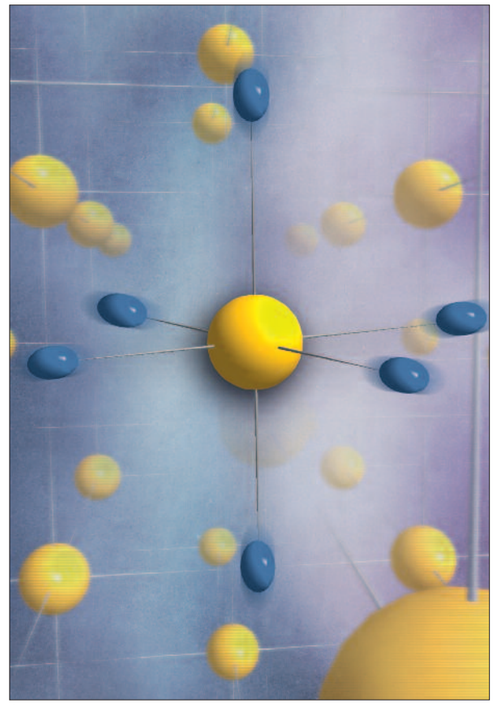
Hydrogen, being the lightest element of the periodic table, is the atom most strongly subjected to such quantum behavior. Indeed, its quantum nature affects structural and physical properties of many hydrogen compounds. An important example is high-pressure ice, where quantum fluctuations of the proton lead to a symmetrization of the hydrogen bonds. Now, new theoretical results suggest that an analogous quantum hydrogen-bond symmetrization occurs in the recently discovered sulfur hydride superconductor, a compound that at high pressure has the highest critical temperature reported for any superconductor so far, 203 K (-70 ºC).

These results were obtained by an international collaboration of researchers from the University of the Basque Country (UPV/EHU) and Donostia International Physics Center (DIPC); Sorbonne Universités–UPMC Université Paris 06; University of Cambridge; Cavendish Laboratory; Jiangsu Normal University; Carnegie Institution of Washington; Jilin University; and Università di Roma "La Sapienza".

The extraordinary discovery of superconductivity at 203 kelvin at 155 gigapascals last year has led to a number of theoretical studies aimed at understanding the origin of the astonishingly high-temperature superconductivity. The overall consensus is that H_2S is metastable at high pressures and its decomposition gives rise to several H-S compounds. Then, superconductivity is believed to occur with H_3S stoichiometry and to be conventional in nature, that is, mediated by the electron-phonon interaction. Calculations that treat hydrogen atoms as classical particles predict that at pressures above 175 gigapascals they sit exactly halfway between two sulfur atoms giving rise to a fully symmetric structure. At lower pressures, though, hydrogen atoms move to an off-center position forming a short H–S covalent bond and a longer H···S hydrogen bond. The main conclusion of this new theoretical study is that, when considering the atoms as quantum particles described by a wave function, the symmetrization pressure for H_3S is lowered by 72 gigapascals, that is, well below 155 gigapascals. Thus, the authors propose that the experimentally measured record superconductivity was observed with the symmetric hydrogen bonds.

According to their calculations, the quantum symmetrization of the hydrogen bond has a tremendous impact on the vibrational and superconducting properties of hydrogen sulfide. Indeed, the first author, Ion Errea, researcher at the University of the Basque Country (UPV/EHU) and Donostia International Physics Center (DIPC) explains that "in order to theoretically reproduce the observed pressure dependence of the superconducting critical temperature, the quantum symmetrization needs to be taken into account".

One of the biggest dreams of science is to achieve superconductivity at room-temperature, and the experiment that last year measured superconductivity at 203 kelvin suggests that room-temperature superconductivity might be possible in other hydrogen-rich compounds. This theoretical study shows that in all these compounds the quantum motion of hydrogen can strongly affect the structural properties, even modifying the chemical bonding, and the electron-phonon interaction that drives the superconducting transition. All those advances in understanding the underlying physics of high temperature superconductivity are a new small step towards achieving the dream.



Structure with symmetric hydrogen bonds induced by the quantum behavior of the protons, represented by the fluctuating blue spheroids.

In order to theoretically reproduce the observed pressure dependence of the record superconducting critical temperature, the quantum symmetrization needs to be taken into account

Ultrafast electronic response of graphene to a strong and localized electric field

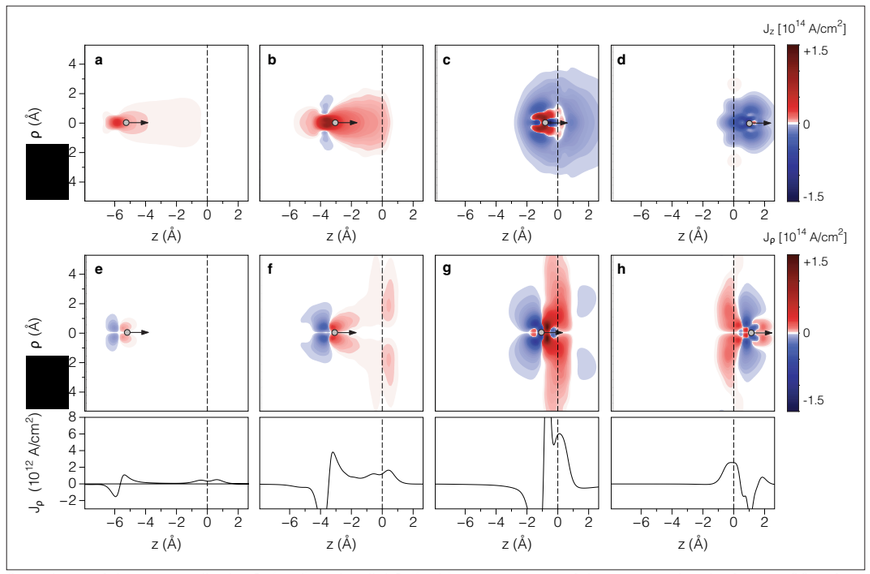
E. Gruber, R.A. Wilhelm, R. Pétuya, V. Smejkal, R. Kozubek, A. Hierzenberger, B.C. Bayer, I. Aldazabal, A.K. Kazansky, F. Libisch, A.V. Krasheninnikov, M. Schleberger, S. Facsko, A.G. Borisov, A. Arnau and F. Aumayr
Nature Communications 7, 13948 (2016)

New experiments and simulations have shown that it is possible for extremely high currents to pass through graphene. This allows imbalances in electric charge to be rapidly rectified without introducing any damage in the graphene layer.

An international research team, formed by both theorists (DIPC-CFM-UPV/EHU Donostia and CNRS Paris) and experimentalists (Helmholtz-Center Dresden-Rossendorf, University of Duisburg-Essen and TU Wien), was able to prove that electrons in graphene are extremely mobile and react very quickly to an ultrahigh electric field. In the experiments, xenon ions, with a particularly high electric charge, impact on a graphene single layer film producing a large number of electrons to be torn away from the graphene in a very precise spot. However, thanks to the theoretical simulations, it was possible to understand that the material is able to replace the electrons within some femtoseconds. This resulted in extremely high currents, which would not be maintained under normal circumstances. Its extraordinary electronic properties make graphene a very promising candidate for future applications in the field of electronics.

The highly charged Xe ions used in the experiments have initial positive charges up to +35, which means that 35 electrons have been removed in the ion source before it collides with the graphene film. However, as it is approaching the film it starts tearing electrons away from the graphene due to its extremely strong electric field. By the time the ion has fully passed through the graphene layer, it has a positive charge of less than +10, compared to over +30 when it started out. The ion is able to extract more than 20 electrons from a tiny area of the graphene film. This means that electrons are now missing from the graphene layer, so the carbon atoms surrounding the point of impact of the xenon ions are positively charged.

Our simulations using time dependent density functional theory (TDDFT) reveal the highly non-linear multi-electron processes responsible for the ultrafast response (few femtoseconds) of graphene electrons to the extremely high electric field produced by the highly charged ion. These processes take place in a few nanometers size spot of the graphene layer, something that translates into extremely high current densities both in the perpendicular and transverse directions to the graphene plane, as shown in the figure below.



Snapshots of the perpendicular J_z (a–d) and radial J_ρ (e–h) components of the current density for q_{in}=20 at four different HCI–graphene distances obtained from TDDFT calculations performed in cylindrical (ρ,z) coordinates with z-axis set along the projectile trajectory perpendicular to the target surface. The figures show that already above the graphene layer electrons are transferred to the approaching HCI and the current density along the direction of motion explains the charge exchange of the HCI. Extremely high transverse current density (f–h) along the graphene layer is obtained. The corresponding profiles (lower panels) show the z-dependent transverse current density averaged over a circle of 10 Å in radius. Values exceeding 10^{12} A cm^{-2} are obtained. The position of the HCI is indicated by a small circle, while the position of the graphene layer by the vertical dashed line.

Our simulations using time dependent density functional theory reveal the highly non-linear multielectron processes responsible for the ultrafast response

Additionally, we show that the experimentally measured keV energy loss experienced by the highly charged ion is transferred to electronic degrees of freedom. Mainly the energy is taken away by ionization of several tens of electrons into the continuum. The holes left in a nm size graphene area as a result of an electron emission and electron capture by the projectile are so quickly neutralized that there is no time to transfer the energy to the lattice producing structural defects.

This extremely high electron mobility in graphene is of great significance for a number of potential applications, like the construction of ultrafast electronic devices or connecting optical and electronic components.

DIPC HIGHLIGHT 2016

Negative dissipation gradients in hysteretic materials

M. Jaafar, O. Iglesias-Freire, P. García-Mochales, J.J. Sáenz, and A. Asenjo
Nanoscale 8, 16989-16994 (2016)

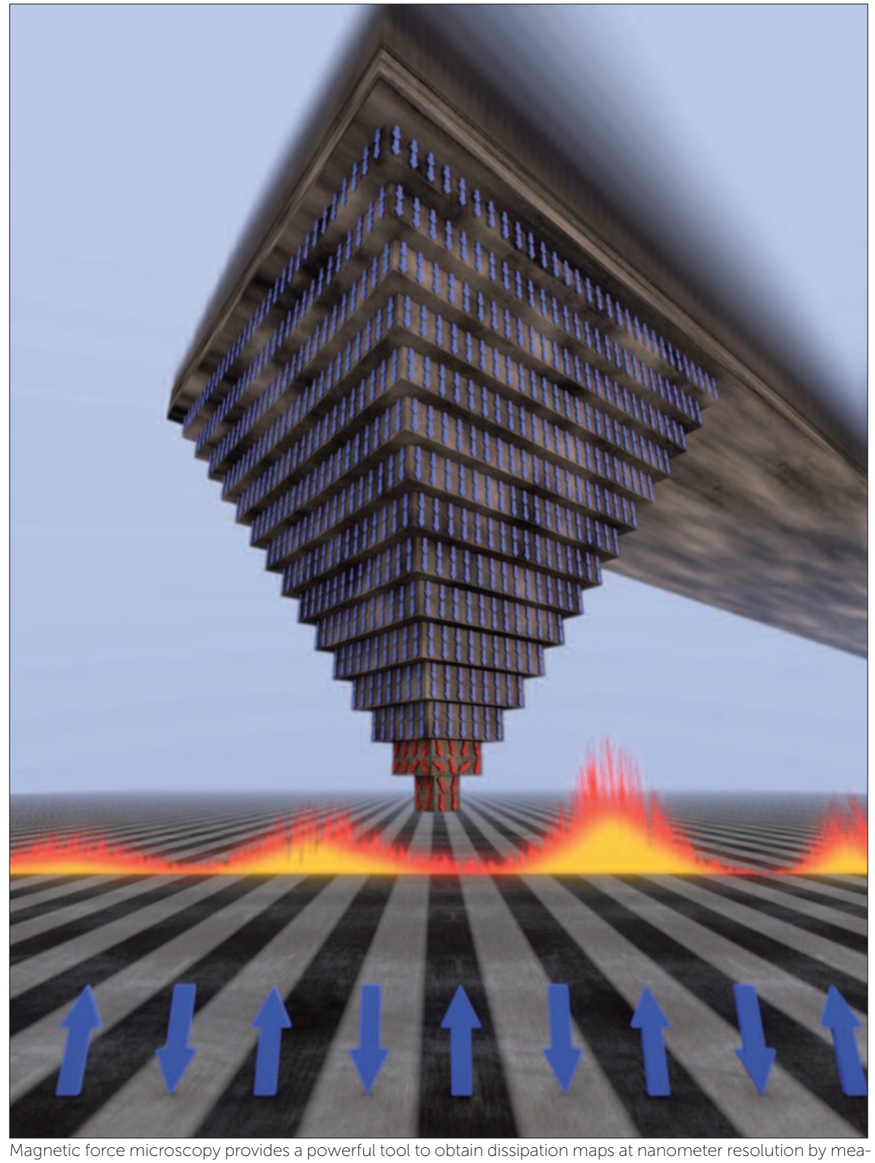
There are many processes of energy dissipation and friction that can be seen in our daily lives. Measuring energy dissipation on the nanoscale is of great interest not only for nanomechanics but also to understand important energy transformation and loss mechanisms.

In particular, dissipation in magnetic and other hysteretic materials is a fundamental problem that plays an important role in numerous applications ranging from design and performance of electronic devices or data storage, to spin-based sensors or biomedical treatments as hyperthermia.

Usually frictional dissipation associated with the relative motion between two bodies, increases as they approach each other, that is, when their mutual interaction is stronger. Now a group of researchers, led by Juan José Sáenz from the Donostia International Physics Center (DIPC) and Agustina Asenjo from the Material Science Institute in Madrid (ICMM-CSIC) describe the unexpected observation of reduction of the energy dissipated as the distance between a magnetic tip and a magnetized sample decreases.

Although at first sight this is a rather counter-intuitive result, it can be explained in relatively simple terms. Two small magnets in front of each other try to always to keep their dipole moments in parallel. When the magnetization of the tip and sample is opposite, some of the spins (that act as a tiny magnets) reorient themselves as the distance decreases, eventually going back as the tip retracts leading to a hysteretic process. Magnetic dissipation can be associated to the energy lost when the electron spins flip their orientation. When the magnetization of the tip and sample is parallel, their mutual interaction is reinforced and the probability of spin flip is reduced as they approach each other. The micromagnetic simulations are in good agreement with the experimentally measured values dissipation, the order of femtowatts.

Increasing the tip-sample magnetic interaction can result in a reduction of magnetic losses



Magnetic force microscopy provides a powerful tool to obtain dissipation maps at nanometer resolution by measuring the tiny amount of energy dissipated by a vibrating tip in the proximity of a sample surface. Measuring the dependence of the energy dissipation with the distance allows separating short-range dissipation processes (adhesion, contact formation, capillary condensation, friction, wear...) from long-range magnetic interactions that depend on the relative orientation of tip and sample spins.

Electron-hole pair effects in polyatomic dissociative chemisorption: water on Ni(111)

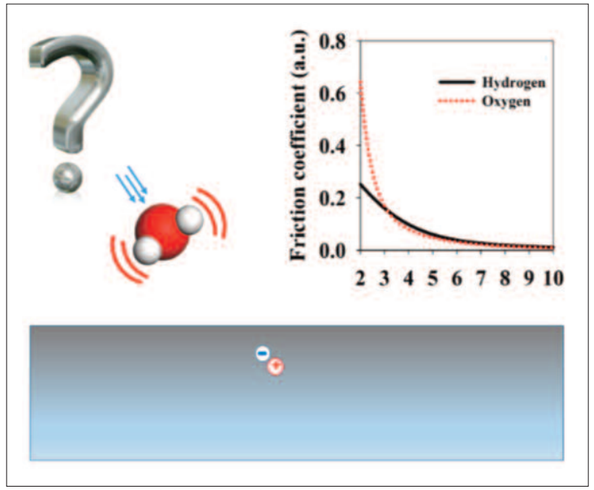
B. Jiang, M. Alducin, and H. Guo
Journal of Physical Chemistry Letters 7, 327-331 (2016)

During World War II the Germans relied on their strong chemical knowledge to overcome the limited access to critical raw materials that the circumstances of the war itself imposed. One of these raw materials was Chilean saltpeter (sodium nitrate), which was the base for explosives. The solution was to use a chemical process designed to produce nitrogen based fertilizers, the Haber-Bosch process, and use it as an initial step for the production of nitrates.

The Haber-Bosch process, $N_2 + 3H_2 \leftrightarrow 2NH_3$, is still the main industrial procedure for the production of ammonia today, and its economic importance is immense, apart from its dramatic and revolutionary impact in agriculture during the 20th century. It was developed in 1908 by Fritz Haber and was developed for industrial use by Carl Bosch. The nitrogen is obtained from liquid air. Before WW2, hydrogen was from water gas and the water gas shift reaction. Now it is obtained by steam reforming of natural gas (methane). All these reactions depend on the interaction and dissociation of a polyatomic gas on a catalyst. Actually, dissociative chemisorption, as it is called, of gas phase molecules on metal surfaces is the initial and often rate-limiting step in many heterogeneous catalysis processes, what explains the great importance of an in-depth understanding of them.

There have been tremendous advances of our knowledge on dissociative chemisorption processes, particularly on mode specificity, namely the different efficacies of vibrational modes of an impinging polyatomic molecule in promoting the dissociation. And one consequence of this new knowledge is that, counterintuitively, dissociative chemisorption processes cannot be described with statistical models, but with quantum mechanical ones.

The generally successful quantum mechanical models used to describe these processes make use of the Born-Oppenheimer approximation, meaning that they assume that, when calculating the motions of electrons, atomic nuclei are in fixed positions. Given the large number of electrons in the metal and zero energy difference among the electronic levels, it should not come as a surprise that a complete separation (adiabaticity) of the electronic and nuclear motions might not always be satisfied. In fact, there is ample evidence of nonadiabaticity in surface processes.



Schematic representation of electron-hole pair excitations induced by a H_2O molecule scattered off a metal surface.

For dissociative chemisorption, the breakdown of the Born-Oppenheimer approximation could significantly affect the dynamics. For example, in the case there were electron-hole (e-h) pairs excitations in the surface of the metal, part of the energy of the impinging molecule could be dissipated to them instead of being used in the bond cleavage.

Now, a team of researchers, including Maite Alducin, from CFM (CSIC-UPV/EHU) and DIPC, report the first explicit examination of the influence of nonadiabatic effects in the surface chemistry of polyatomic molecules, namely the dissociative chemisorption of water on Ni(111). The breakdown of the Born-Oppenheimer approximation in the dissociative chemisorption dynamics, as mentioned, is considered by the researchers as the interaction of the impinging molecule with low-energy electronic excitations in the metal. Such an interaction is approximately represented in classical molecular dynamics by a friction term. Friction models have been successfully used to describe a wide range of nonadiabatic processes on surfaces. To simplify the calculations, the atoms in the molecule are treated as independent, something that has been recently shown to be accurate enough. A second approximation is used, as the atomic friction coefficients are computed considering that the embedding electron density at the atomic coordinate controls the magnitude of the friction force experienced by the molecule.

The calculations show that the nonadiabatic effects due to surface excitons are small and have little impact on the mode specificity of the dissociative chemisorption process of water. However, important caveats of the model are worth noting. Despite the strong evidence that the independent atom approximation is a reasonable one, the complete neglect of the molecular nonadiabatic couplings is likely to introduce some errors. This is a crucial issue to be investigated in the future.

DIPC HIGHLIGHT 2016

Quantifying electronic band interactions in van der Waals materials using angle-resolved reflected-electron spectroscopy

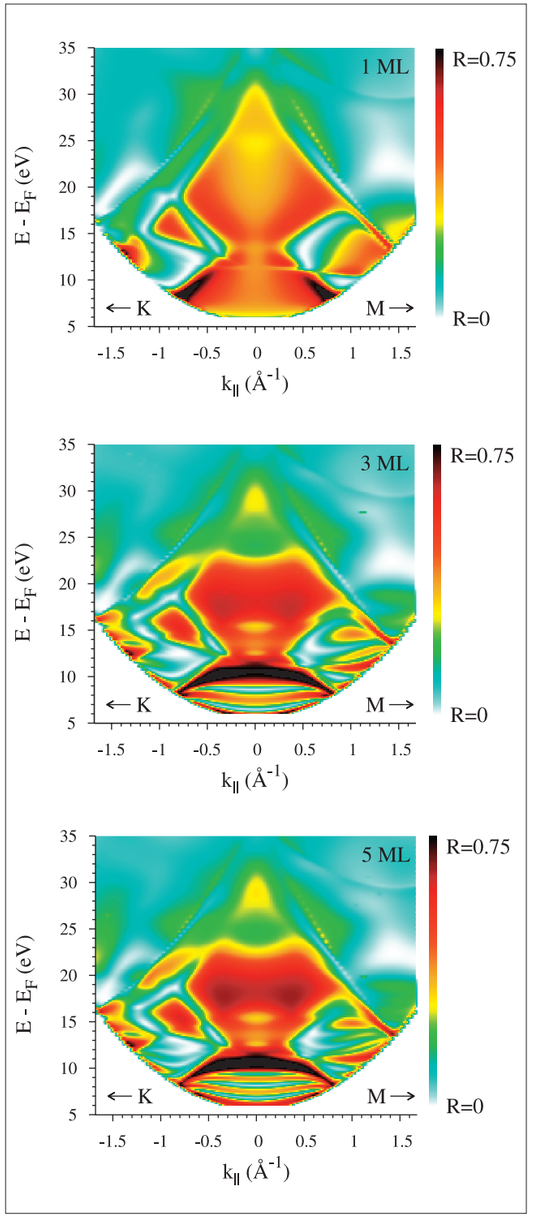
J. Jobst, A.J.H. van der Torren, E.E. Krasovskii, J. Balgley, C.R. Dean, R.M. Tromp, and S.J. van der Molen
Nature Communications 7, 13621 (2016)

A crystal can be thought of as composed of atomic layers stacked at regular intervals, and it is of fundamental importance to understand how the three-dimensional properties of the bulk crystal emerge from the properties of the planar layers. The van der Waals materials, like multi-layer graphene or boron nitride, offer a natural platform for studying the interaction between the individual layers. The experiment on the diffraction of electrons at very low energies is the most direct way to study the interlayer conductance in great detail, i.e., with energy and angular resolution.

An experimental method of angle-resolved reflected-electron spectroscopy developed by the group of Sense Jan van der Molen (Leiden University) was combined with an *ab initio* scattering theory for stand-alone films developed by Eugene Krasovskii (DIPC) to make a definitive statement that the hexagonal boron nitride (hBN) and graphene do not interact over a wide energy range, despite their very similar electronic structure.

In the experiment, the electrons of very low energies are shone at a stack of few-layer graphene on hBN at different angles, and the probability of being reflected is measured. The energy-momentum distribution of the transmitted current shows how the band structure is formed with growing number of layers, see figure. Stacking together n identical layers gives rise to $n - 1$ transmission resonances (which in the limit of an infinite crystal evolve into a conduction band). The study shows that for hBN and graphene the transmission resonances exist in the same energy range. Thus, in view of the similar interlayer distance in hBN and graphene and the similar scattering potential wells of the layers one may expect the stacking of few-layer graphene on bulk hBN to produce no transmission resonances. However, rapid oscillations of the transmission were clearly observed in the experiment and reproduced and explained by the theory. This finding is crucial because the efficient electronic decoupling of the layers underlies the high carrier mobility in graphene-hBN heterojunctions.

This work presents new insight into the graphene-hBN system. It proves the angle-resolved reflected-electron spectroscopy to be an efficient tool for studying layered materials and demonstrates the predictive power of the augmented-plane-waves based scattering theory.



Revealing the electronic structure of heterostructures of graphene and hexagonal boron nitride by electron reflection

Calculated energy-momentum distribution of the reflectivity of three thin films of hexagonal boron nitride: 1, 3, and 5 monolayers (ML) for the wave vector of the incident electron pointing in the directions $\bar{\Gamma}\bar{K}$ and $\bar{\Gamma}\bar{M}$ of the 2D Brillouin zone. Some characteristic features of the reflection map are seen already for the 1 ML film, which reveals their purely 2D origin. For 3 and 5 MLs the transmission resonances at low energies are clearly seen.

Force-induced tautomerization in a single molecule

J.N. Ladenthin, T. Frederiksen, M. Persson, J.C. Sharp, S. Gawinkowski, J. Waluk, and T. Kumagai
Nature Chemistry 8, 935-940 (2016)

An international team of researchers from Donostia International Physics Center, Fritz-Haber Institute of the Max Planck Society, University of Liverpool, and the Polish Academy of Sciences has shown a new way to operate a single-molecule switch by applying an external force. The combined experimental and theoretical work, published in *Nature Chemistry*, opens a unique capability for studying mechanical activation and processing at the single-molecule level, elementary reactions that are involved in many important biological functions and are crucial in molecular devices.

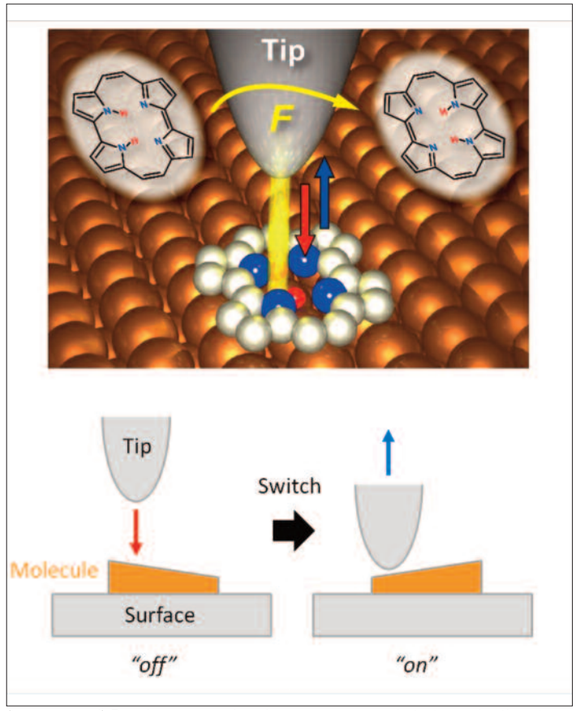
Everybody knows the force that is required to activate a light switch on a wall – a finger is enough. But how much force do you need to apply if the device was dramatically reduced to the "nanoscale world", that is, how much force do you need to operate a "single-molecule switch"? This fundamental question is related not only to basic science but also to potential future applications of molecular devices.

Researchers at Donostia International Physics Center, San Sebastian (Basque Country, Spain), Fritz-Haber Institute of the Max Planck Society, Berlin (Germany), University of Liverpool, (UK) and Polish Academy of Sciences, Warsaw (Poland) have succeeded in activating in a controlled manner a "single-molecule switch" by the force from the atomically-sharp needle of a state-of-the-art scanning probe microscope.

The experimental and theoretical study, reported in the prestigious journal *Nature Chemistry*, demonstrates that an intramolecular hydrogen atom transfer can be triggered in a suitable organic molecule adsorbed on a surface by bringing the sharp metallic tip sufficiently close. The reaction, called tautomerization, is important in organic chemistry and molecular biology and also an interesting phenomenon for molecular electronic devices.

The researchers could not only quantify the force needed to operate their tiny switch, a porphycene molecule on a copper surface, but also reveal that the switching can be only induced at a very specific positions of the tip over the molecule, with a spatial resolution of a fraction of a chemical bond length, namely about 0.02 nanometers. Furthermore, they demonstrated the significance of the "chemical reactivity" of the tip apex in the force-induced process as the molecule cannot be switched when the apex of the needle is decorated by a single xenon atom – an inert element that lacks the required chemical reactivity.

Takashi Kumagai at FHI-MPG, who conceived this study, constructed the experimental setup in which an oscillating needle of a combined atomic force and scanning tunneling microscope is approached within a few atomic distances to the molecule. The switching showed up as a characteristic feature in the frequency shifts upon approach of the tip and was also confirmed by changes at the atomic-scale images



Triggering intramolecular hydrogen atom transfer in porphycene on Cu(110)

(upper panel) Porphycene molecule on a copper substrate under the atomically sharp needle (tip). (lower panel) Schematic illustration of the operation of the switch.

by simultaneously scanning the tip over the molecule. It was measured that the force required was about one nano-Newton, which is a little less than the force needed to break a typical covalent bond between two atoms.

The research team also carried out extensive computer simulations in order to elucidate the atomistic mechanism behind the force-induced switching. The simulations successfully reproduced the experimental results and provided atomistic description on the operation of the single molecule switch. Thomas Frederiksen, Ikerbasque Research Professor at DIPC explains that "our calculations revealed that the tautomerization, that is the switching, occurs by a reduction of its energy activation barrier upon approach of a metallic tip. However, the behaviour dramatically changes with a xenon-terminated tip and no tautomerization could be induced because of its inertness and softness".

The researchers emphasize that the studied force-induced reaction involving changes in the reaction pathway resembles an elementary step in catalytic processes. Therefore, their results also provide a novel strategy to gain a deeper atomistic insight into catalytic reactions, leading to a new control of chemistry at the atomic level.

Concentrated solutions of single-chain nanoparticles: a simple model for intrinsically disordered proteins under crowding conditions

A.J. Moreno, F. Lo Verso, A. Arbe, J.A. Pomposo, and J. Colmenero
Journal of Physical Chemistry Letters 7, 838-844 (2016)

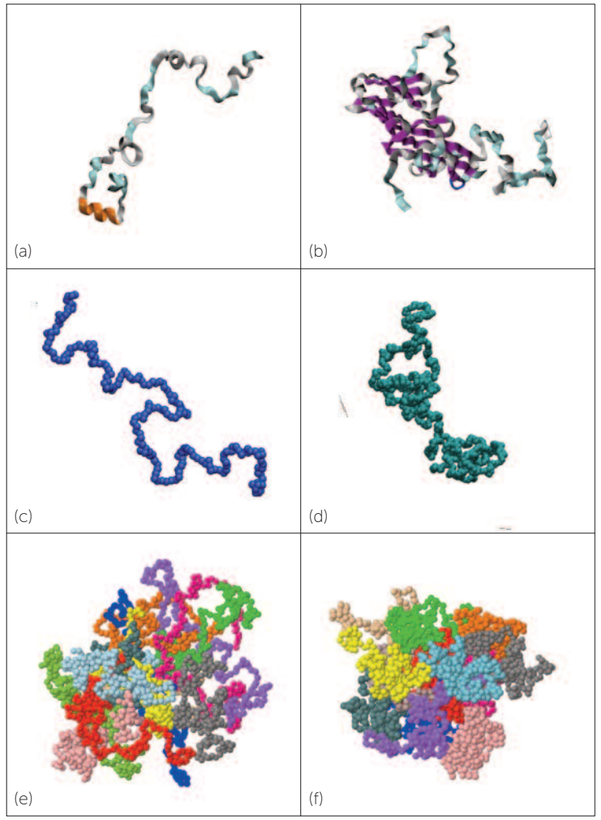
By means of computer simulations and small-angle neutron scattering (SANS), we investigate solutions of single-chain nanoparticles (SCNPs). The conformational properties of the SCNPs share basic ingredients with intrinsically disordered proteins (IDPs), as topological polydispersity, generally sparse conformations, and locally compact domains. Our results propose a general scenario for the effect of steric crowding on IDPs: collapse from sparse conformations at high dilution to crumpled globular conformations in concentrated cellular environments.

Single-chain nanoparticles (SCNPs) are an emergent class of soft nano-objects with promising applications in e.g., nanomedicine, biosensing, bioimaging, or catalysis. They are synthesized through intramolecular cross-linking of polymer precursors. A detailed simulation analysis of their conformations reveals that they share structural ingredients with intrinsically disordered proteins (IDPs), as topological polydispersity, compact domains and sparse regions.

IDPs are highly abundant in eukaryotes. Their biological function is founded on their internal dynamics and flexibility, enabling them to respond quickly to environmental changes and to bind with different cellular targets. As a direct consequence of their malleability, the structural, dynamic and associative properties of IDPs can be affected by macromolecular crowding *in vivo*, substantially differing from the observations *in vitro* at highly dilute conditions.

We exploit the structural analogies between SCNPs and IDPs and investigate the conformational properties of SCNPs in concentrated solutions. SCNPs provide a model system that shares universal structural features with IDPs and is free of specific interactions, allowing to investigate separately the purely steric, excluded-volume contributions to crowding. For this purpose, we combine large-scale simulations of a generic bead-spring model for solutions of SCNPs, and small-angle neutron scattering (SANS) experiments on real systems, covering the whole concentration range from infinite dilution to melt density. We analyze the role of the internal degree of disorder of the SCNP on its collapse behavior under macromolecular crowding. We find that crowding leads to collapsed conformations of SCNPs resembling those of the crumpled globular class. This behavior is already found at volume fractions (about 30 %) that are characteristic of crowding in living cells.

Our results in SCNPs propose a universal scenario for IDPs: steric crowding in cell environments leads IDPs to adopt crumpled globular conformations. The well-known transition from self-avoiding to random coil (Gaussian) conformations in linear polymers is only a particular case, taking place in the limit of fully disordered IDPs.



Simulation snapshots. (a): IDP in the limit of full disorder. (b): IDP with a compact domain. (c): Polymer chain. (d): SCNP. (e): Concentrated solution of polymer chains, showing Gaussian conformations. (f): Concentrated solution of SCNPs, showing crumpled globular conformations.

Our results suggest that intrinsically disordered proteins under steric crowding adopt crumpled globular conformations

Single-chain polymer nanoparticles provide a model system that shares universal structural features with intrinsically disordered proteins and is free of specific interactions

High temperature ferromagnetism in a $GdAg_2$ monolayer

M. Ormaza, L. Fernández, M. Ilyn, A. Magaña, B. Xu, M.J. Verstraete, M. Gastaldo, M.A. Valbuena, P. Gargiani, A. Mugarza, A. Ayuela, L. Vitali, M. Blanco-Rey, F. Schiller, and J.E. Ortega
Nano Letters 16, 4230-4235 (2016))

To understand the exotic solid state magnetic properties observed in nanoscale ferromagnets, or the quantum phenomena that arise at ferromagnet/semiconductor and ferromagnet/superconductor interfaces, new model systems and complex materials are needed. Now a team of researchers from DIPC and other institutions may have found one.

Fundamental research on magnetism, as well as many potential nanotechnology applications on spintronics, relies on the ability to interface magnetic materials with superconductors, topological insulators, and organic or inorganic semiconductors. To achieve this, tailoring magnetic properties on structurally robust substrates is crucial. The survival of the long-range magnetic order upon interface formation is a basic requirement, and that is the reason why, besides structural stability and chemical inertness, substrate materials with strong ferromagnetism, i.e., high Curie temperatures (above which ferromagnetism is suppressed), are sought. Although high Curie temperatures are readily found at the surface of some elementary ferromagnetic materials, interfacing them very often results in intermixing and finally in the lack of structural and magnetic control.

Rare-earth/noble metal monolayer alloys grown on noble metal surfaces represent an interesting alternative as magnetic templates. This is because, besides their structural stability, their nanoscale modulation offers a way to drive the growth of nanosized structures. In the case of the gadolinium-gold (Gd-Au) combination, by varying the Gd coverage, nanoscale patterns can be tuned. These have been utilized as structurally robust templates for the self-organization of cobalt (Co) nanodot arrays, which show tunable magnetic coupling with the alloyed substrate.

Given the variety of rare earth elements and their exotic magnetism, the observations made on $GdAu_2$ encouraged the team led by F. Schiller and J.E. Ortega, from DIPC and the Materials Physics Center CSIC-UPV/EHU, to carry out a thorough search combining different rare earth elements and noble metals. Recently, in collaboration with Andrés Ayuela and María Blanco, they completed a detailed experimental and theoretical investigation, utilizing scanning tunneling microscopy (STM), X-ray magnetic circular dichroism (XMCD), magneto-optic Kerr effect (MOKE), angle-resolved photoemission (ARPES), and theoretical density-functional theory (DFT) calculations, in order to unveil the electronic structure and magnetic properties of the gadolinium-silver alloy, $GdAg_2$, in parallel with the structurally identical $GdAu_2$. They noted important and interesting differences between these two alloys.

$GdAg_2$ also revealed optimal templating properties, namely structural stability and nanoscale modulation. In addition, the $GdAg_2$ monolayer itself exhibited excellent crystal quality and ferromagnetic order. The researchers found a high Curie temperature of 85 K, which was particularly intriguing when compared to

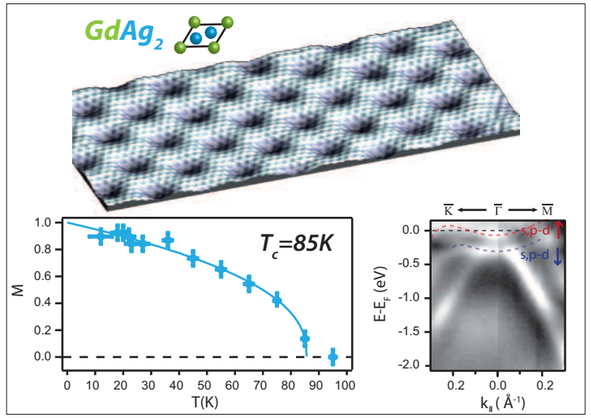


Figure 1. (Top) STM micrograph of the two-dimensional $GdAg_2$ surface compound. (Left) Remanent magnetization values at different temperatures extracted from MOKE loops measured at zero applied field. The Curie temperature of the monolayer (85 K) has been derived from the fit of the MOKE data. (Right) Experimental electron band structure measured by ARPES.

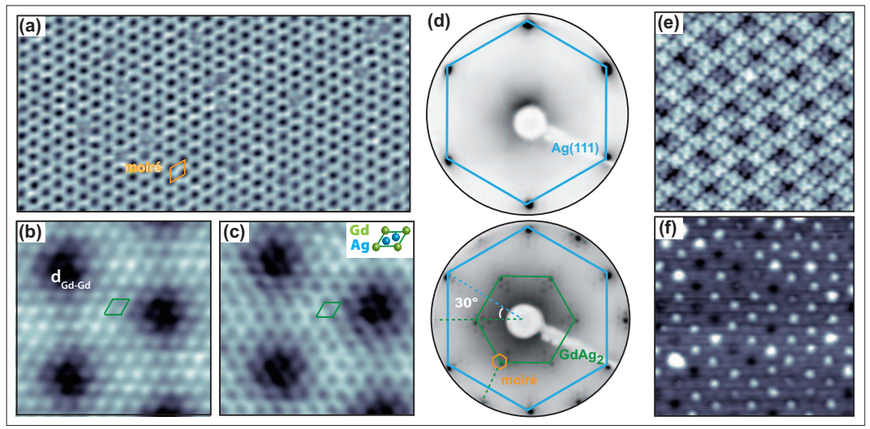


Figure 2. (a,b,c) STM micrographs of the two-dimensional $GdAg_2$ surface compound measured by different STM imaging settings. They reveal the characteristic long range moiré modulation and the atomic resolution of the monolayer (unit cell marked in green). (d) Low-energy electron diffraction patterns of Ag(111) and $GdAg_2$ monolayer. STM micrographs of (e) 1ML of H_2Pc and (f) Co nanodots grown on $GdAg_2$ confirm the good templating properties of this surface.

the low value of 19 K of $GdAu_2$. Such difference could not be predicted using previous knowledge of the parent bulk compounds, since these are antiferromagnets with similarly low Neel temperature. Yet this surprising behavior could be explained by the ARPES and DFT results. These prove that the Curie temperature depends on the hybrid gadolinium/noble-metal band-filling in each case, in particular, on the presence of a high density of in-plane Fermi energy states that mediate RKKY coupling, which is maximum for Ag, but minimum for Au.

On-surface engineering of a magnetic organometallic nanowire

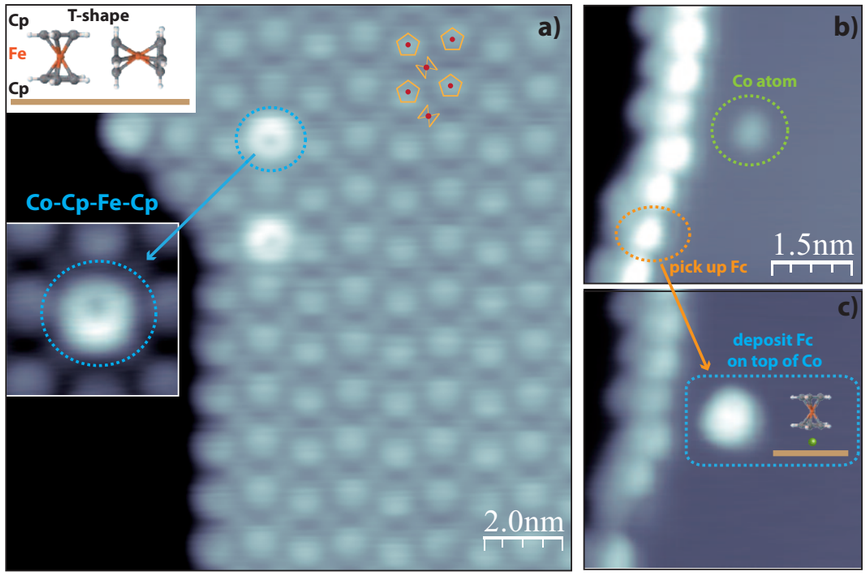
M. Ormaza, R. Robles, N. Bachellier, P. Abufager, N. Lorente, and L. Limot
Nano Letters 16, 588-593 (2016)

Using atoms and molecules to assemble the ultimate computing device is an actively pursued goal. The stakes are high but low-cost, high-efficiency and whopping performances are simply too good to ignore. One stumbling block in atomic-scale devices is how you actually interconnect them. Atomic and molecular wires seem to be a good option. Additionally, molecular wires can be active. They can perform tasks thanks to their internal structure. In the above work, the authors show one way of creating a hybrid atomic-and-molecular wire using single-atom manipulation, and characterize its interesting electronic and magnetic properties.

Metallocenes are small molecules composed of two C_5H_5 rings (one C—H short of benzene) that encapsulate a metallic atom (usually Fe, Co or Ni). This tiny sandwich has some amusing properties. Their bonds are incredibly sturdy, so it is quite difficult to compress it. However, the sandwich structure allos some easy parallel displacement of one of the "buns" (C_5H_5) with respect to the other one. But its electronic properties are more interesting. The pentadienyl rings (the "buns") capture one extra electron, becoming charged. Hence the metallic atoms are in valence II (having lost two electrons). Additionally, the rings imposed an interaction on the metallic atom distorting its electronic structure along one given axis. The consequence is that the remaining electronic structure is confined to distorted d orbitals of the metallic atom, inducing sometimes magnetism. Or not. In the case of Fe, which is naturally magnetic with a sizeable 4 Bohr magnetons of intrinsic magnetic moment, the magnetism is totally quenched. Indeed, ferrocene (C_5H_5-Fe-C_5H_5 or $FeC_{10}H_{10}$) has no magnetic moment. Although if we could increase the distortion of the molecule along the molecular axes, the splitting among electronic states is reduced and a high-magnetic-moment state of 4 Bohr magnetons is retrieved. However, the molecules are not easy to distort and under isolation, the state in the low-magnetic-moment configuration. Cobaltocene ($CoC_{10}H_{10}$) has 1 Bohr magneton, and nickelocene ($NiC_{10}H_{10}$) has 2 Bohr magnetons. There is ample room for inducing magnetism just by changing the metallic core, while most molecular chemical properties are preserved.

Over the years many researchers have been seduced by this family of molecules, metallocenes, because one can pile them up creating wires. Such molecular wires are almost a 1-D array of magnetic moments and can be excellent to produce highly spin-polarized electronic currents. However, this is difficult to achieve with Fe-based metallocenes. For this reason, the authors of the above work tried to create a hybrid system combining the non-magnetic ferrocene with magnetic Co atoms. First, they studied experimentally the assembly of a one-molecule high layer of ferrocenes on a copper surface. By means of scanning tunneling microscopy (STM) they were able to understand the observed complex molecular pattern. The experimental work assisted by theory showed that the ferrocene assembly previously published in the literature was not accurate. It was found that in the metallocene assembly horizontal as well as vertical ferrocenes are present. In fact, the T-shape interaction between the cyclopentadienyl rings of both, horizontal and vertical, molecules are responsible of the stabilization of the layer.

Next, Co atoms were added to the ferrocene structure, producing a novel Co-Cp-Fe-Cp molecular wire which can be easily identified in the STM images (fig. a). DFT calculations were crucial to identify the position of the Co atom, showing the higher stability of Co atom when placed underneath the molecules and in contact with the Cu surface. This was rationalized by the higher coordination of an otherwise reactive atom. Remarkably, the calculation showed that the magnetic moment of the Co atoms decreased a little, while the Fe atom as well as the Cp rings become slightly magnetized. This was experimentally checked by studying the conductance signal at zero bias and very low temperatures. In the presence of a magnetic impurity, the wave function of a metal becomes correlated which yields a strong resonance at the Fermi energy if thermals effects do not destroy the coherence of the wavefunction. The consequence is a peak at zero bias in the conductance at very low temperature. This is called the Kondo effect. Our hybrid atom-molecule system displayed the Kondo effect, revealing the existence of a small magnetic moment at the system's position. The most amazing finding of this work is that it was possible to produce an isolated Co-Ferrocene wire by using a controlled manipulation procedure (fig. b-c), giving rise to same results as for the wire within the molecular layer. The agreement between theory and experiment was excellent, giving strong support to the idea that these systems can become of technological interest soon.



(a) STM image of a self-assembled monolayer of ferrocene (Fc) molecules on Cu surface. The layer is stabilized by the T-shape interaction between both, vertical and horizontal; molecules. Deposition of Co atoms gives rise to new molecules (higher contrast in the image), in which the Co atom is placed underneath a vertical molecule within the layer. Building process of an isolated Co-ferrocene: (b) a ferrocene (Fc) molecule at a step edge is picked up with the tip of the STM and (c) is afterwards deposited on top of a Co atom by a molecular tip-atom contact.
Image sizes: (a) 10x10nm^2, (b-c) 8x8nm^2. Image parameters: (a) -30mV, 500pA, (b-c) -1V, 100pA.

Substrate-independent growth of atomically precise chiral graphene nanoribbons

D.G. de Oteyza, A. García-Lekue, M. Vilas-Varela, N. Merino-Díez, E. Carbonell-Sanromà, M. Corso, G. Vasseur, C. Rogero, E. Guitián, J.I. Pascual, J.E. Ortega, Y. Wakayama, and D. Peña
ACS Nano 10, 9000-9008 (2016)

Graphene nanoribbons (GNRs), are strips of graphene with ultra-thin width (<50 nm). Graphene ribbons were introduced as a theoretical model by Mitsutaka Fujita and coauthors to examine the edge and nanoscale size effect in graphene.

GNRs are very interesting structures, partly due to their attractive electronic properties. Those properties vary dramatically with changes in the nanoribbon's atomic structure in terms of width, crystallographic symmetry, dopant heteroatoms, and edge termination. Moreover, the electronic properties can be modulated even further by the appropriate design of GNR heterostructures. This enormous tunability of electronic properties is thus extremely promising for next-generation nanoelectronic and optoelectronic devices. However, the high susceptibility of those properties to minimum changes in the GNR structure also indicates the stringent need for atomic precision in GNR synthesis (Figure 1). With the advent of bottom-up synthesis, increasingly high hopes are being placed on this approach, but the field is still in its infancy. Actually, although a large pool of GNRs with different edge orientations, widths, or heteroatoms (and heterostructures) should be possible, only a few GNRs have been successfully synthesized with the required selectivity and precision so far.

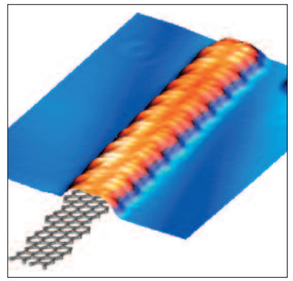


Figure 1. Schematic representation of the chiral GNRs synthesized in this work, with an overimposed scanning tunneling microscopy image revealing its atomic precision.

To date, the most widely studied nanoribbon is the GNR with seven dimer lines across its width (7-AGNR) that grows from 10,10'-dibromo-9,9'-bianthracene (reactant *1* in Figure 2) in a multistep reaction, including dehalogenation, polymerization (also known as Ullmann coupling), and cyclodehydrogenation. The synthesis of 7-AGNR has been shown to work reproducibly on substrates such as Au(111), Au(110), or Ag(111). Surprisingly, the same reactant 1 designed to render AGNRs turned out to form chiral (3,1)-GNRs on Cu(111) (Figure 2).

The problem was that the careful consideration of the reactions involved indicate that this is a very system-specific reaction mechanism not translatable to other substrates, based on the surface-catalyzed, selective activation of particular C–H bonds. Nevertheless, those results have inspired the work of a team coordinated

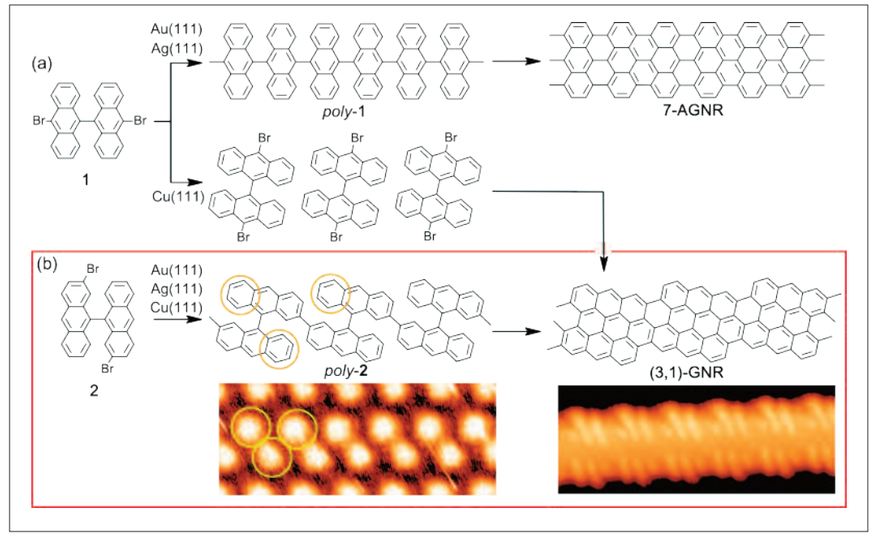


Figure 2. (a) Schemes of the chemical reactions of precursor 1 on various metallic surfaces. On Au(111) and Ag(111), it affords armchair GNRs. On Cu(111), it affords chiral (3,1)-GNRs. (b) de Oteyza et al. (highlighted with the red line) report the transformation of reactant 2 into chiral GNRs independently of the substrate [Au(111), Ag(111), and Cu(111)]. Associated STM images are shown for poly-2 after initialpolymerization by Ullmann coupling, as well as for the final (3,1)-GNR after cyclodehydrogenation, both on Au(111). Steric hindrance causes poly-2 to be nonplanar. The high parts (circled inyellow) are correspondingly marked in the polymer's wireframe structure above.

by Dimas G. de Oteyza, Ikerbasque professor working at DIPC and CFM (CSIC-UPV/EHU) and Diego Peña, from CIQUS and USC, that includes researchers from these institutions plus UPV/EHU, CIC nanoGune, and Yutaka Wakayama from MANA. The team reports in ACSNano that they have found a way of growing, independently of the substrate, chiral GNRs that are atomically precise.

Inspired by the system-specific growth of (3,1)-GNRs on Cu(111) from precursor *1*, the researchers designed an alternative building block *2* (Figure 2) that renders the same (3,1)-GNRs but now independently of the substrate material. This has been proven on Au(111), Ag(111), and Cu(111), revealing additional advantages of the use of this monomer in the growth of selective and atomically precise GNRs, as is the substantially increased length of the resultant GNRs and the low processing temperature required for their formation.

Furthermore, the growth process has been followed in detail combining core level spectroscopy, scanning tunneling microscopy, and density functional theory calculations, providing a clear correlation between the spectroscopic fingerprints and the different reaction processes, as well as revealing the unusual absence of a metastable metal-organic intermediate preceding the covalent polymerization in the Ullmann coupling process on Ag(111). The substantial GNR lengths achieved and the low processing temperature required to complete the reaction grant this reactant extremely interesting properties for potential applications.

DIPC HIGHLIGHT 2016

Peculiar all-metal σ-aromaticity of the $[Au_2Sb_{16}]^{4-}$ anion in the solid state

I.A. Popov, F.-X. Pan, X.-R. You, L.-J. Li, E. Matito, C. Liu, H.-J. Zhai, Z.-M. Sun, and A.I. Boldyrev
Angewdante Chemie International Edition 55, 15344-15346 (2016)

A set of lanthanide antimony clusters that represent the first isolable compounds containing an all-metal antiaromatic ring has been prepared by treating lanthanide benzyl complexes with the Zintl cluster complex K_5Sb_4 in pyridine solvent and then isolating the anions as potassium cryptand salts. The electronic structure analysis reveals the antiaromatic character of the rhombic Sb_4 rings that serve as ligands to the lanthanide metals. This set of lanthanide clusters, $[Ln(Sb_4)_3]^{3-}$ (Ln=La, Y, Ho, Er and Lu), represent the first example of isolable inorganic antiaromatic compounds.

***Aromaticity* is a ubiquitous term in chemistry** referring to the cyclic electron delocalization that leads to energy stabilization, bond length equalization, and exalted magnetic properties, among other particular features. Its antonym is *antiaromaticity*, which was coined by Breslow to refer to situations where "electronic delocalization is destabilizing". In the past years, the synthesis of new aromatic compounds of inorganic nature has shaken the traditional concept of aromaticity, now extended to include new species such all-metal aromatic clusters. These days, there are a number of new inorganic species commonly referred as aromatic, whereas there are very few antiaromatic molecules that are not organic.

The group of Prof. Sun's from the Changchun Institute of Applied Chemistry, has synthesized a collection of all-metal clusters, $[Ln(Sb_4)_3]^{3-}$ (Ln=La, Y, Ho, Er, or Lu), that contain three Sb_4 antiaromatic units. These clusters have been prepared by treating lanthanide benzyl complexes with the Zintl cluster complex K_5Sb_4 in pyridine solvent and then isolating the anions as potassium cryptand salts. X-ray analysis revealed that each Sb_4 ring is stabilized by a η^4-interaction with the lanthanide metal, but the electronic distribution of each ring structure and the aromaticity of the Sb_4 units was unclear.

The groups of Prof. Boldyrev and Dr. Eduard Matito, an Ikerbasque Research Fellow working at the Chemistry Faculty of UPV/EHU and the DIPC, focused on analyzing the electronic structure of these clusters using computational calculations. In the $[La(\eta 4\text{-}Sb_4)_3]^{3-}$ cluster computational calculations suggest a formal assignment of La^{3+} and three Sb_4^{2-} units within the cluster, in agreement with simple electron count rules. However, the electronic arrangement of the Sb_4^{2-} unit within the $[La(\eta^4\text{-}Sb_4)_3]^{3-}$ cluster is very different from the isolated Sb_4^{2-} molecule. Upon coordination with La, the electronic structure of the Sb_4^{2-} units changes drastically its electronic distribution, resulting in a less aromatic Sb_4^{2-} unit. The strong η^4-interaction hinders the internal ring delocalization that exists in the aromatic free Sb_4^{2-} moiety. Comparisions

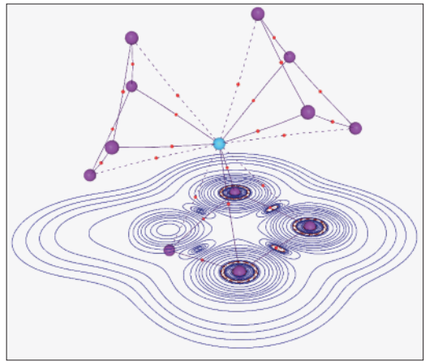


Figure 1. Isocountour plot of the Laplacian of the electron density in the Sb_4 antiaromatic unit within the $[La(\eta^4\text{-}Sb_4)_3]^{3-}$ cluster.

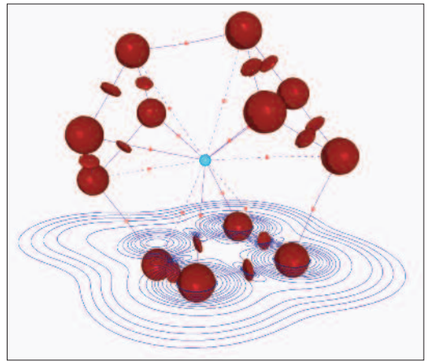


Figure 2. The isosurface plot of the Laplacian of the electron density ($\nabla^2\rho(r)$=-0.001) reveals the bonding interactions in the Sb_4 antiaromatic units of the $[La(\eta^4\text{-}Sb_4)_3]^{3-}$ cluster.

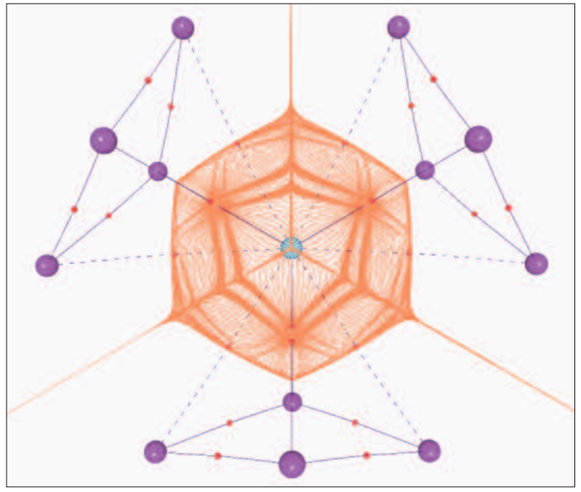


Figure 3. The atomic boundary of La atom in the $[La(\eta^4\text{-}Sb_4)_3]^{3-}$ cluster is a polyhedric structure with edges pointing to the Sb_4 units.

with non-aromatic and antiaromatic organic analogs, deems to conclude that the Sb_4^{2-} unit within the $[La(\eta^4\text{-}Sb_4)_3]^{3-}$ cluster has a rather antiaromatic character, similar to the quintessential antiaromatic organic compound, cyclobutadiene. These results were published in *Angewandte Chemie* and highlighted in *Chemistry & Enginnering News*.

This set of lanthanide clusters, $[Ln(Sb_4)_3]^{3-}$ (Ln=La, Y, Ho, Er and Lu), represent the first example of isolable inorganic antiaromatic compounds. Further advances of aromaticity and antiaromaticity are important in grasping the properties of metal clusters, bulk metals and alloys, which are valuable for making thin-film electronic materials.

Imaging single-molecule reaction intermediates stabilized by surface dissipation and entropy

A. Riss, A. Pérez-Paz, S. Wickenburg, H.-Z. Tsai, D.G. de Oteyza, A.J. Bradley, M.M. Ugeda,
P. Gorman, H.S. Jung, M.F. Crommie, A. Rubio, and F.R. Fischer
Nature Chemistry 8, 678-683 (2016)

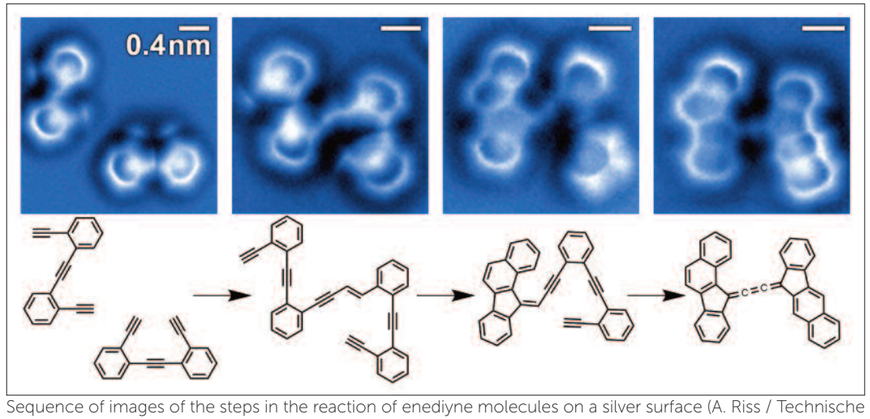
An international team of researchers has for the first time imaged and identified the bond configuration of the intermediates in a complex sequence of chemical transformations of enediyne molecules on a silver surface and has resolved the microscopic mechanisms that account for their behaviour.

One of the long-standing goals being pursued by chemists has been to succeed in following and directly visualising how the structures of molecules change when they undergo complex chemical transformations. Reaction intermediates, which are highly unstable substances that form in different steps in a reaction before the products are obtained, are particularly difficult to identify and characterise owing to their short lifetimes. Getting to know the structure of these intermediate species may be very helpful in understanding the reaction mechanisms and, what is more, could have a great impact on the chemical industry, materials science, nanotechnology, biology and medicine.

Now for the first time, researchers have imaged and resolved the bond configuration of the reactants, the intermediates and final products of a complex, organic reaction at the single-molecule level. The prestigious journal *Nature Chemistry* has published this research.

The work was carried out by the research groups led by Felix R. Fischer and Michael F. Crommie (University of California at Berkeley and Lawrence Berkeley National Laboratory), and by Angel Rubio (Professor at the UPV/EHU, leader of the UPV/EHU's Nano-Bio Spectroscopy Research Group, and Director of the Max Planck Institute for the Structure and Dynamics of Matter in Hamburg). The Ikerbasque Research Professors Dimas G. Oteyza, researcher at Donostia International Physics Center (DIPC) and Miguel Moreno Ugeda from CIC Nanogune played a significant role in the experiments conducted at Berkeley.

The team has obtained the images of the chemical structures associated with different steps in the reaction cascade involving multiple steps of enediyne molecules on a silver surface, using non-contact atomic force microscopy (nc-AFM) with a particularly sensitive tip: it uses a very fine needle that can detect the smallest bumps on an atomic scale (in a way not unlike reading in Braille) as it absorbs a carbon monoxide molecule that acts like a "finger" on the text to increase its resolution.



Sequence of images of the steps in the reaction of enediyne molecules on a silver surface (A. Riss / Technische Universität München).

The precise identification of the bond configuration of the intermediate species "has made it possible to determine the intricate sequence of chemical transformations along the reaction mechanism from reactants via intermediates to end products," explained Ángel Rubio, the UPV/EHU professor, "and at the same time unravel the microscopic mechanisms behind that intricate dynamical behaviour".

Stabilizing the intermediates

By combining the latest advances in numerical calculus and the classical analytical models that describe the kinetics of sequential chemical reactions, an area that explores the speed of the reactions and the molecular events taking place in it has been proven. So to explain the stabilization of the intermediates, it is not enough just to consider their potential energy, it is essential to bear in mind the energy dissipation and the changes in molecular entropy, which measures how far a system is organised. The surface, and in particular the interaction of the extremely unstable intermediates with the surface, play a key role for both the entropy and the dissipation of energy, which highlights a fundamental difference between the surface-supported reactions and gas-phase or solution chemistry.

Such detailed understanding achieved though the synergy between the imaging of the chemical reactions of a molecule and the latest advances in computer modelling constitutes a fundamental milestone in the analysis of chemical reactions. All this new knowledge may open up countless hitherto unexplored fields: future designs and optimizations of heterogeneous catalytic systems, development of novel synthetic tools applied to carbon-based nanotechnology, as well as biochemical and materials science applications.

Quantum mechanical description of raman scattering from molecules in plasmonic cavities

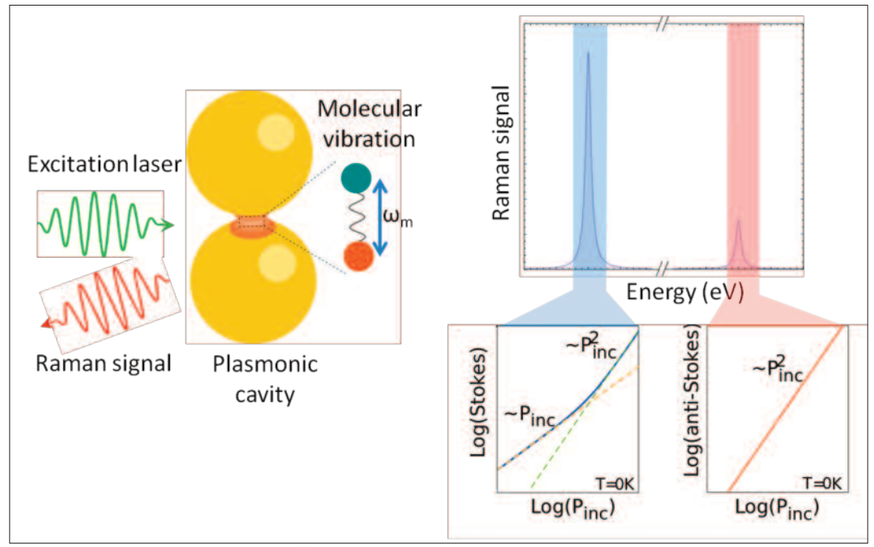
M.K. Schmidt, R. Esteban, A. González-Tudela, G. Giedke, and J. Aizpurua
ACS Nano 10, 6291-6298 (2016)

When light interacts with a molecule a coherent transfer of energy between light and the vibrations of the molecule can occur, in a process known as Raman scattering. In the Stokes Raman process, a photon loses a fraction of its energy as it induces the molecule to vibrate. The opposite, anti-Stokes, process is also possible, where the energy released by the decay of a vibrational state is gained by a photon.

By measuring the energy of the scattered photons it is thus possible to obtain information about the vibrations of the molecule, which provides important chemical information for identification and fingerprinting of the molecular species. Notably, although Raman processes are usually very inefficient, they can be boosted enormously when the molecules are coupled with optical resonances in metallic nanoparticles associated to the excitation of localized surface plasmons. The resulting Surface-Enhanced Raman Spectroscopy (SERS) has been traditionally understood using classical and phenomenological models, but a quantum treatment can lead to important new insights about the coherence and quantum properties of the systems.

The key to SERS is that the plasmonic resonances can localize light very strongly, which leads to a very efficient interaction with a nearby molecule. When this coupling is modeled using quantum electrodynamics, SERS is described in the same manner as the optical response of a very rich family of physical systems known as optomechanical (OM) resonators. In fact, the analogy can be seen as more than a purely formal one. Typical OM systems exploit the coupling between a photonic resonance and a macroscopic mechanical mode, as for example when the mirror in a Fabry-Pérot cavity can oscillate resonantly. In SERS, the plasmon plays the role of the photonic mode, and the molecular vibration corresponds to the mechanical oscillation. Thus, SERS can be seen as a molecular OM system.

A collaboration between the DIPC and Centro de Física de Materiales (CSIC-UPV/EHU) in San Sebastián and the Max-Planck-Institute for Quantum Optics in Germany has shown, in a paper published in ACS Nano, that this description allows to gain considerable insight into the dynamics of the SERS process. Notably, it allows to model from fundamental principles a range of phenomena that are not considered in most typical treatments. These effects include non-linearities in the Stokes signal due to phonon-stimulated emission, strong correlations of the emitted photons and a complex dependence of the emitted signal on the temperature and the frequency and intensity of the illumination.



On the left: Schematics of a typical SERS setup, where a molecule is positioned in the hot-spot of a plasmonic dimer nanoantenna. On the right: Typical Raman scattering spectrum, where the central peak describing elastic scattering is not shown and the two side-peaks denote the inelastic Stokes and anti-Stokes scattering processes. The panels underneath show the typical dependence of the Stokes (left) and anti-Stokes (right) scattering on the power of the incident laser Pinc at low temperatures. The phonon stimulated processes described in this paper boost the intensity of the Stokes scattering, providing a quadratic dependence on Pinc for intense lasers.

These effects include non-linearities in the Stokes signal due to phonon-stimulated emission, strong correlations of the emitted photons and a complex dependence of the emitted signal on the temperature and the frequency and intensity of the illumination

Such phenomena might be observed in state-of-the-art experiments, and may even have already been inadvertently revealed in some recent measurements. Furthermore, the quantum treatment of SERS can have an impact not only for spectroscopy studies, but also on the study of general OM phenomena, because the values of the vibrational and photonic parameters involved in the plasmon-molecule coupling are very different to those typically found in other OM configurations. This study thus opens optomechanics to a new regime of interactions.

The ω-SQUIPT as a tool to phase-engineer Josephson topological materials

E. Strambini, S. D'Ambrosio, F. Vischi, F.S. Bergeret, Yu. V. Nazarov, and F. Giazotto
Nature Nanotechnology 11, 1055-1059 (2016)

The Josephson effect is a macroscopic manifestation of quantum interference. It consists of the flow of a current without dissipation that takes place when two superconductors are coupled through a tunneling barrier or a non-superconducting metal. In the latter case the superconducting correlations can penetrate the normal metal and this acquires superconducting properties such as the ability of sustain a supercurrent and a gap in the density of states (DOS). The amplitude of this gap can be controlled by the macroscopic phase difference between the superconducting leads in the junction. In particular, the induced gap closes when the phase difference equals to π.

Josephson junctions based on multiple superconductor terminals offer an unique opportunity to tailor non-trivial quantum states in nanoscale weak links and enlarge the dimension of the phase space in which the opening and close of the induced gap occurs.

In a collaboration between the theory groups of Sebastian Bergeret at the CFM-DIPC and Yuli Nazarov at the Delft University of Technology, together with the experimental group of Francesco Giazotto in Pisa, a three-terminal Josephson interferometer has been analyzed. Tunneling spectroscopy measurements reveal transitions between gapped (that is, insulating) and gapless (conducting) states that are controlled by the phase configuration of the three superconducting leads connected to the junction. These transitions are topological: a gapless state necessarily occurs between two gapped states of different topological indices, in much the same way that the interface between two insulators of different topologies is necessarily conducting. The topological numbers that characterize such gapped states are given by superconducting phase windings over the two loops that form the Josephson interferometer. As these gapped states cannot be transformed to one another continuously without passing through a gapless condition, they are topologically protected. The findings of this work are pivotal for enabling phase engineering of different and more sophisticated artificial topological materials.

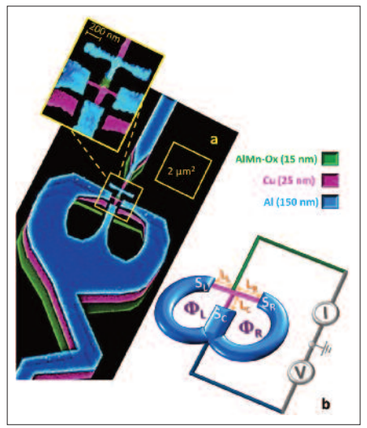


Figure 1. The multi-terminal Jospehson junction investigated (the ω-SQUIPT). The normal metal is Cu (red) and the superconducting terminals are made of Al (blue).

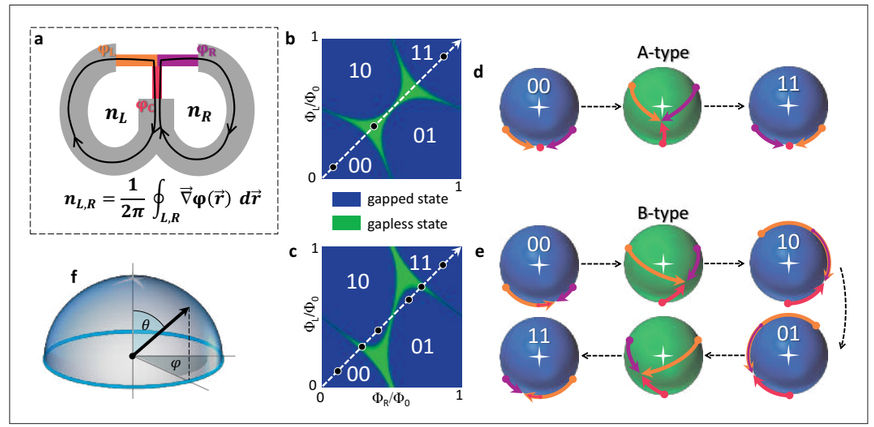


Figure 2. (a) Sketch of the double-loop interferometer with the geometric paths used to determine the topological index (n_L,n_R). These are defined by the closed line integral of the gradient of the superconductor phase φ(r) along the left (n_L) and right (n_R) loops. (b,c) The density of states at the Fermi energy calculated for two different ω-SQUIPTs. The blue areas indicate the insulating (gapped) states classified by the topological index in (a). (d,e) Vectorial representation of the evolution of the topological state along the lines in (b) and (c) accessible in our experiment.

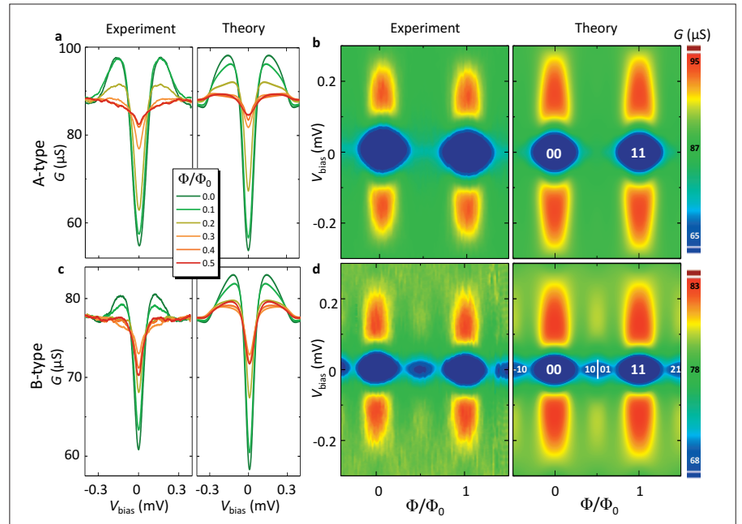


Figure 3. Comparison between the tunnelling conductance G versus V_{bias} measured at 30 mK and calculated for selected values of Φ (= $Φ_L$ = $Φ_R$) for both types of ω-SQUIPTs in Figure 2.

DIPC HIGHLIGHT 2016

Large-scale sublattice asymmetry in pure and boron-doped graphene

D. Yu. Usachov, A.V. Fedorov, O. Yu. Vilkov, A.E. Petukhov, A.G. Rybkin, A. Ernst, M.M. Otrokov, E.V. Chulkov, I.I. Ogorodnikov, M.V. Kuznetsov, L.V. Yashina, E. Yu. Kataev, A.V. Erofeevskaya, V. Yu. Voroshnin, V.K. Adamchuk, C. Laubschat, and D.V. Vyalikh
Nano Letters 16, 4535 - 4543 (2016)

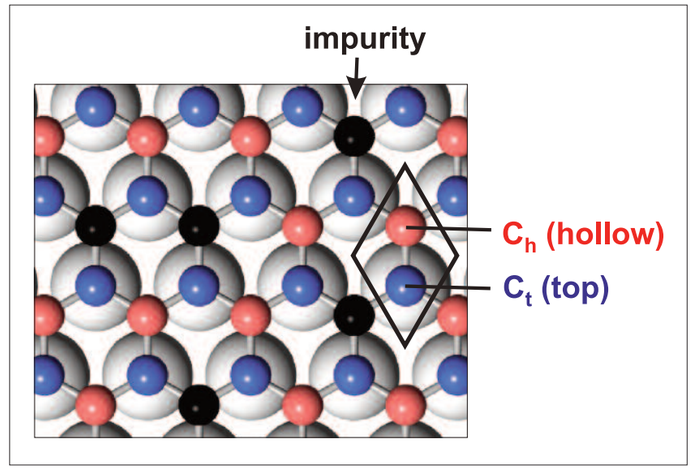
Among the astonishing properties of graphene, a high mobility of the charge carriers has placed this material into the focus of intensive research efforts, aimed at developing high-speed graphene-based electronic devices. The first device of this family, a graphene field-effect transistor (GFET), still remains a promising candidate for applications in flexible electronic circuits.

An essential handicap that limits the performance of planar GFETs is the absence of a band gap in the graphene electronic structure. The gap is necessary to reach a high on/off current ratio. In the recent past, several approaches have been developed for opening and controlling the gap. These methods include adsorption of atoms and molecules, but the material still remains gapless.

A promising approach for the graphene band gap engineering is to introduce a large-scale sublattice asymmetry. When the foreign atoms become randomly embedded only in one graphene sublattice, the resulting system possesses a notable band gap improving the transport properties of conventional GFETs. Experimental observation of the discussed unbalanced sublattice doping is quite elusive, though. Doping asymmetry was detected with scanning tunneling microscopy (STM) in nitrogen-doped graphene, grown on a Cu(111) substrate. It was proposed that a possible mechanism responsible for breaking of the sublattice symmetry is related to oscillations in the local density of states driven by the impurities.

Now an international team of researchers, that includes Mikhail M. Otrokov, Evgueni V. Chulkov and Ikerbasque professor Denis V. Vyalikh from DIPC and cooperation partner Dmitry Yu. Usachov from Saint Petersburg State University, using photoelectron diffraction and spectroscopy has demonstrated a selective incorporation of boron impurities into only one of the two graphene sublattices. According to performed *ab initio* calculations, such boron-doped graphene possesses a band gap that can be precisely controlled by the dopant concentration. B-graphene with doping asymmetry is, thus, a novel material, which is worth considering as a good candidate for electronic applications.

The approach is illustrated in the figure. When doped graphene is synthesized on a crystal face with hexagonal structure and well-matched lattice constant, a strong symmetry breaking may occur. This happens when one sublattice, marked as C_t, is adsorbed on top of the substrate atoms of Co(0001), while the other sublattice C_h occupies the hollow sites.



Concept of using a single-crystalline lattice-matched substrate as a pattern for unbalanced sublattice doping of graphene. In the top-hollow interface structure impurities may occupy sites in one sublattice.

B-graphene with doping asymmetry, a novel material, is worth considering as a good candidate for electronic applications

The early studies of the graphene/Co(0001) system showed that graphene is formed by randomly oriented domains sticked to the metallic substrate. However, it was recently shown that under certain conditions well-oriented graphene can be grown. Such an interface, and particularly its geometry, remain poorly explored, though. In the present work, the researchers unveil the structural properties of the graphene/Co(0001) interface and show that the cobalt substrate is very well suitable for large-scale unbalanced doping of graphene with substitutional boron impurities.

In the well-oriented graphene/Co(0001) system, one sublattice of carbon is placed above Co atoms, while the second one occupies the hollow sites. This unique property of the interface makes cobalt an ideal substrate to be used as a platform for the synthesis of doped graphene with impurities incorporated in one of the two C-sublattices. This is conclusively demonstrated by the example of the B-graphene/Co(0001) system, in which boron impurities preferably substitute carbon atoms in one sublattice, located above the hollow sites of the metal substrate.

The *ab initio* calculations predict that such asymmetrically doped graphene should have an intrinsic band gap and the width of the gap can be controlled by the dopant concentration. Thus, B-graphene with demonstrated doping asymmetry becomes a novel material, which is worth considering as a good candidate for applications in GFETs and other graphene-based electronics.

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282 Anisotropic effective interactions and stack formation in mixtures of semiflexible ring polymers.
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Soft Matter 12, 4805 (2016).

283 Dielectric relaxation of polymers: segmental dynamics under structural constraints.
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284 Tunable slow dynamics in a new class of soft colloids.
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286 Resolubility of image-potential resonances.
Höfer U, and Echenique PM.
Surface Science 643, 203 (2016).

287 Adsorption of polyiodobenzene molecules on the Pt(111) surface using van der Waals density functional theory.
Johnston K, Pekoz R, and Donadio D.
Surface Science 644, 113 (2016).

288 Rotation assisted diffusion of water trimers on Pd{111}.
Ranea VA, and de Andres PL.
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289 Cyclopropanation reactions catalysed by dendrimers possessing one metalloporphyrin active site at the core: linear and sigmoidal kinetic behaviour for different dendrimer generations.
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Book Chapters

1 **Dynamical processes in open quantum systems from a TDDFT perspective: resonances and electron protoemission.**
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Density Functional Methods for Excited States Book Series: Topics in Current Chemistry 368, pp. 219-271. Springer Int. Publishing AG (2016).

2 **Optoelectronic and transport properties of gapped graphene.**
Gumbs G, Huang D, Iurov A, Gao Bo.
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3 **Simulation of dimensionality effects in thermal transport.**
Donadio D.
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4 **Recent progress on nonlocal graphene/surface plasmons.**
Horing NJM, Iurov A, Gumbs G, Politano A, Chiarello G.
Low Dimensional and Nanostructured Material and Devices: Properties, Synthesis, Characterizations, Modelling and Applications Nanoscience and Technology, pp. 205-237,
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DIPC COMMUNITY

Pictured here is part of the DIPC Community at the headquarters in Donostia / San Sebastián on September 23rd, several days before the opening of Passion for Knowledge 2016.

DIPC HEADQUARTERS
DONOSTIA / SAN SEBASTIÁN
23 SEPTEMBER 2016

Researchers

Fellows Gipuzkoa

Dr. Rubén Esteban Llorente
11/03/2013–31/12/2016
Quantum plasmonics.

Dr. Maia Garcia Vergniory
01/06/2013–04/09/2016
Electronic and magnetic properties in ordered and disordered topological insulators.

Dr. Peter Koval
25/11/2013–Present
Development of MBPT with localized orbitals.

Dr. Aitzol Garcia Etxarri
01/11/2014–Present
Nanophotonics theory.

Senior Positions

Dr. Irina Sklyadneva
Electron-phonon coupling in the 3D topological isolators and Weil semiconductors as well as and in ultrathin lead and indium films on the Si substrate (superconductivity).

Prof. Vladimiro Mújica Hernandez
Charge and spin transfer at nano-interfaces. Reformulation of Marcus theory using the molecular polarizability as fundamental variable.

Postdoctoral Positions

Dr. Stepan Tsirkin
State University of Tomsk, Russia
06/12/2012–04/09/2016
Magnetic proximity effect in the layered structures.

Dr. María de Gracia Retamosa Hernández
Facultad de Química, UPV/EHU, Donostia / San Sebastián, Spain
01/07/2013–31/01/2016
Remote structural effects in unnatural amino acids.

Dr. Mikhail Otrokov
State University of Tomsk, Russia
17/07/2013–31/12/2016
Topological insulators.

Dr. Iosune Arrastia Basalo
Facultad de Química, UPV/EHU, Donostia / San Sebastián, Spain
01/08/2013–Present
Multiple spin state reactivity in Fe-containing complexes and enzymes.

Dr. Elena Formoso Estensoro
Università della Svizzera Italiana, Lugano, Switzerland
01/02/2014–31/12/2016
Unveiling biochemical relevant structural conformations of the aluminum cation amyloid-beta peptide complex.

Dr. Federica Lo Verso
Material Physics Center, MPC, Donostia / San Sebastián, Spain
01/02/2014–Present
Structure and dynamics of complex materials based on polymers.

Dr. Rémi Pétuya
Institut des Sciences Moléculaires, Université Bordeaux, France
01/10/2014–30/09/2016
Characterization of structural and electronic properties of molecular overlayers on metal surfaces.

Dr. Romain Dupuis
CEMES/CNRS, Toulouse, France
10/12/2014–Present
Computational studies on calcium silicate hydrates.

Dr. Guillaume Vasseur
Institut Jean Lamour, Université de Lorraine-CNRS, France
05/01/2015–08/08/2016
Physics and chemistry of curved crystal surfaces.

Dr. Joseba Alberdi Rodriguez
Facultad de Informática, UPV/EHU, Donostia / San Sebastián, Spain
01/07/2015–Present
Morfokinetics: development of computational techniques for the analysis of CVD growth of new 2D materials.

Dr. Marta Pelc
Nicolaus Copernicus University, Torun, Poland
01/12/2015–Present
Topological defects on carbon like nanostructures.

Dr. Omjyoti Dutta
University of Arizona, Tucson, Arizona, USA
01/01/2016–Present
Quantum matter and quantum simulations at the interface of optics and solid state physics.

Dr. Daniel Martinez Tong
Université Libre de Bruxelles, Belgium
11/01/2016–Present
Local dielectric spectroscopy by AFM. Application to polymer based materials.

Dr. Pablo Aguado Puente
CIC nanoGUNE
15/02–30/06/2016
Coupling of ferroic nanoscale films with interfacial two dimensional electron gases in oxides.

Dr. Mathias Ljungberg
Phillips Universität Marburg, Germany
01/04/2016–Present
Model calculations of solid organic/inorganic interface.

Dr. Carlos Garcia Fernandez
Instituto Superior de Ciencias y Tecnologías Nucleares, La Habana, Cuba
20/04/2016–Present
Development of transport methods based on Wannier function.

Dr. Mario Zapata Herrera
Universidad de los Andes, Bogotá, Colombia
01/07/2016–Present
Quantum and classical approaches to the optical response of metallic nanostructures.

Dr. Pawel Nita
Marie Curie-Sklodowska University, Lublin, Poland
01/08/2016–Present
Functional materials synthesized by surface-supported chemistry under vacuum.

Dr. Jon Iñaki Mujika
Facultad de Química, UPV/EHU, Donostia / San Sebastián
16/08/2016–Present
Molecular dynamics of membrane structure.

Dr. Aleksander Terentjev
Instituto Nanoscienze-CNR, Euromediterranean Center for Nanomaterial Modelling and Technology (ECMT), Lecce, Italy
01/09/2016–Present
Time dependent density functional theory beyond the local density approximation.

Dr. Jorge Budagosky Marcilla
Universidad de Zaragoza, Spain
01/10/2016–Present
Computational solid state spectroscopy.

Dr. Victor Escobedo Bermudez
Universidad de Salamanca, Spain
01/10/2016–Present
Literature and science.

Dr. Nuno De Sousa
Universidad Autónoma de Madrid, Spain
08/11/2016–Present
Light scattering, emission rates and optical forces in colloidal suspensions.

Dr. Maxim Ilin
Materials Physics Center CSIC-UPV/EHU, Donostia / San Sebastián, Spain
16/12/2016–Present
Upgrade of MOKE setup to add up the capability for as-susceptibility measurements.

PhD Students

Anton Xose Brion Rios
18/02/2016-Present
Theoretical study on the molecular adsorption and self-organization on substrates of different nature.

Dino Novko
25/09/2013–Present
Non-adiabatic effects in the interaction of metal surfaces with atoms and small molecules.

Oihana Galparsoro Larraza
01/10/2013–30/09/2016
Phonon and electron excitations in diatom abstraction from metallic surfaces.

Bernhard Kretz
09/06/2014–Present
Electronic and transport properties of graphenic nanostructures.

Lucía Ortega Álvarez
12/01/2015–Present
Structure and dynamics of silica filled rubber compounds.

Natalia Koval
21/01/2015–19/01/2016
Time-dependent density functional theory calculations of the energy loss of particles in metallic media.

Néstor Merino Díez
01/09/2015–Present
Tema de investigación: Functional materials synthesized by surface-supported chemistry under vacuum.

Mattin Urbieta
01/01–10/04/2016
Plasmonics of metallic nanoparticles and hybrid nanostructures.

Mohamed Ahmed Nosir
01/01–30/12/2016
Theoretical study of the dynamics of nitrogen atoms and molecules interacting with iron surfaces.

Jon Lafuente Bartolomé
01/01/2016–Present
Relativistic corrections and spinorial structure of the response function in 2D systems.

Bogusz Bujnowski
01/04/2016–Present
Quantum transport in hybrid structure with semimetals, excitonic insulators and superconductor.

Federico Marchesin
14/07/2016–31/12/2016
Ab initio plasmonics using LCAO basis sets.

Jordan Ochs
01/10/2016–Present
Synthesis of cyclic polymers.

Jorge Olmos Trigo
01/10/2016–Present
Theory and modelling of topological photonic materials.

Evgenia Rusak
01/10–16/12/2016
Quantum description of plasmonic systems and their coupling with single emitters.

Cristina Sanz Fernandez
01/10–14/12/2016
Light emission and propagation in all-dielectric photonic structures.

Olatz Uranga Barandiaran
15/11/2016–Present
Theoretical and computational studies of excited states in molecules and aggregates.
Functional materials synthesized by surface-supported chemistry under vacuum.

Internships

Daniel Camacho Piris
Facultad de Informatica, UPV/EHU, Donostia / San Sebastián, Spain
01/06–31/08/2016
Batch system management

Gonzalo Oyarzabal Insausti
Facultad Informática, UPV/EHU, Donostia / San Sebastián, Spain
01/06–31/08/2016
Cluster monitorization.

Olatz Romeo Amiama
Facultad de Informática, UPV/EHU, Donostia / San Sebastián, Spain
01/06–31/08/2016
Unatended instalation.

Alvaro Martinez Dominguez
Facultad de Ciencia y Tecnología, Leioa, UPV/EHU, Spain
06/06–05/08/2016
Light scattering and optical forces on nanoparticles.

Asier Insausti Gonzalez
Facultad de Ciencia y Tecnología, UPV/EHU, Leioa, Spain
13/06–12/08/2016
Massless Kane fermions in the topological insulator HgCdTe.

Javier López Piqueres
Universidad Autónoma de Madrid, Spain
20/06–19/08/2016
Trapping matter with nano-structures.

Unai Muniain Caballero
Facultad de Ciencia y Tecnología, UPV/EHU, Donostia / San Sebastián, Spain
20/06–19/08/2016
Atomic scale engineering of graphene nanostructures.

Alvaro Cuartero Gonzalez
Universidad Autónoma de Madrid, Spain
24/06–23/08/2016
Optical antennas to control light at the nanoscale.

Lucia Gonzalez Rosado
Universidad Autónoma de Madrid, Spain
27/06–27/08/2016
Topological invariants of Majorana fermions in a chain of magnetic atoms.

Rodrigo Asensio Perea
Facultad de Ciencia y Tecnología, UPV/EHU, Leioa, Spain
01/07–31/08/2016
Optical antennas to control the angular momentum of light.

Juan Reino González
Universidad Autónoma de Madrid, Spain
04/07–04/09/2016
Development of density functionals in DFT.

Nerea Jiménez Irurzun
Facultad de Quimica, UPV/EHU, Donostia / San Sebastián, Spain
01/08–30/09/2016
Topological gels based on cyclic polymers.

Sofia Sanz
Universidad Autónoma de Madrid, Spain
05/09–31/10/2016
Quantum transport in nanoscale devices.

Igor Cortés Cejudo
Facultad de Informática, UPV/EHU, Donostia / San Sebastián, Spain
03/10–31/01/2017
Virtual machines cluster installation.

Miriam Rico Medina
Facultad de Informática, UPV/EHU, Donostia / San Sebastián, Spain
03/10–31/01/2017
Energy saving system for the computer clusters.

Ikerbasque Research Professors

Prof. Andreas Heidenreich
Computer simulations of nanoplasma formation, Coulom explosions and nuclear fusion induced by ultraintense and ultrashort laser pulses. Computer simulations of pump-probe signals.

Prof. Andrey Kazanskiy
Investigation of subfemto atto second processes in gases and solids caused by ultrashort laser pulses. Investigation of dynamics of electrons in suface and image states of noble metal and their interaction with adsorbates.

Prof. Eugene Krasovskii
Electronic structure of nanosystems, surfaces and interfaces. Attosecond time resolved photo-electron spectroscopy to study the dynamics of electronic excitations. Full dielectric function of bulk crystals, surfaces and two dimensional nanostructures. Development of new computational methods of the density funtional theory.

Prof. Mario Piris Silveira
Energy functional method development. Computational modelling of semiconductor nanocluster and molecular solid phases and polymorfism.

Prof. Slawomir Grabowski
Analyses of intra-and intermolecular interactions in the gas phase, ab initio and DFT calculations as well as the use of the other theoretical methods as for example Quantum theory of atoms in molecules and natural bond orbitals approach. Studies on crystal structures of organic and organometallic compounds, analyses of different Lewis acid.Lewis base interactions (mostly hydrogen bonding) influencing geometries of species constituting crystals and influencing arrangement of molecules and/or ions in crystals, the use of theoretical methods for these analyses as well as statistical methods as for example factor analysis.

Prof. Vyacheslav Silkin
Ultrafast dynamics of the one-particle and collective electronic excitations in metals and their surfaces. The study of electronic excitations at adsorbates on metal surfaces.

Prof. Thomas Frederiksen
Nanoelectronics - theory and simulation.

Prof. Geza Giedke
Quantum Information and Quantum Optics: Implementations of QIP in atomic and solid-state systems.

Prof. Dimas Garcia de Oteyza Fieldman
Physical chemistry phenomena in organic materials and organic-inorganic interfaces.

Prof. Juan José Saenz Guitierrez
Light scattering in colloidal suspensions.

Prof. Fabienne Barroso Bujans
Novel complex-shaped cyclic polymers, from synthesis to physical properties. Devices and nanodevices based on cyclic polymers/graphene hybrid materials.

Ikerbasque Research Fellows

Dr. Arantzazu Garcia Lekue
01/11/2012–Present
Modeling electron transport at the nanoscale. Theoretical investigation of electron processes at nanostructured surface.

Dr. María José Cabrera San Félix
01/11/2012–Present
Molecular level understanding of the interaction of molecules (particularly water) with surfaces and their self-assembly to form extended structures. Electronic and structural properties of clean and decorated surfaces: surface reconstructions and chemical reactivity.

Dr. Dario Bercioux
01/10/2014–Present
Quantum transport in nanostructures.

DIPC Associates

Prof. Javier Aizpurua CSIC
Dr. Maite Alducin CSIC
Dr. Ignacio Arganda-Carreras UPV/EHU
Prof. Andrés Arnau UPV/EHU
Prof. Emilio Artacho CIC nanoGUNE
Dr. Andrés Ayuela, CSIC
Prof. Rolindes Balda UPV/EHU
Dr. Aitor Bergara UPV/EHU
Dr. Sebastian Bergeret CSIC
Dr. Maria Blanco UPV/EHU
Dr. Igor Campillo Euskampus
Dr. David Casanova UPV/EHU
Dr. Miguel Ángel Cazalilla CSIC
Prof. Eugene Chulkov UPV/EHU
Prof. Juan Colmenero UPV/EHU
Prof. Fernando Cossio UPV/EHU
Dr. Fernando Delgado UPV/EHU
Dr. Ricardo Díez Muiño CSIC
Prof. Pedro Miguel Echenique UPV/EHU
Dr. Asier Eiguren UPV/EHU
Dr. Ion Errea UPV/EHU
Prof. Joaquín Fernández UPV/EHU
Dr. Idoia García de Gurtubay UPV/EHU
Dr. Maia Garcia Vergniory UPV/EHU
Prof. Francisco José García Vidal UAM
Dr. Miguel Angel Gosalvez UPV/EHU
Dr. Iñaki Juaristi UPV/EHU
Dr. Aritz Leonardo UPV/EHU
Dr. Xabier Lopez UPV/EHU
Dr. Nicolás Lorente CSIC
Dr. Eduard Matito UPV/EHU
Dr. Jon M. Matxain UPV/EHU
Dr. Jose M. Mercero UPV/EHU
Dr. Angel Moreno CSIC
Prof. Enrique Ortega UPV/EHU
Prof. Juan Ignacio Pérez UPV/EHU
Prof. José Maria Pitarke UPV/EHU
Prof. Yuri Rakovich UPV/EHU
Dr. Elixabete Rezabal UPV/EHU
Prof. Alberto Rivacoba UPV/EHU
Dr. Celia Rogero CSIC
Prof. Ángel Rubio UPV/EHU
Dr. Daniel Sánchez Portal CSIC
Dr. Ane Sarasola UPV/EHU
Dr. Frederik Schiller CSIC
Dr. Gustavo Ariel Schwartz CSIC
Prof. Ivo Souza UPV/EHU
Prof. Jesus M. Ugalde UPV/EHU
Prof. Lucia Vitali UPV/EHU
Dr. Nerea Zabala UPV/EHU

Visiting Researchers

Long visits

Dr. Vitaly Golovach
CNRS Grenoble, France
01/11/2012–31/10/2017
Electronic properties at the nanoscale.

Dr. Mathias Ljunberg
Laboratoire ondes et matière d'Aquitaine (LOMA) - CNRS, Talence, France
16/04/2014–16/04/2016
First principles calculations of complex oxides.

Dr. Rafael Grande Aztatzi
Cinvestav, Centro de Investigación y Estudios Avanzados del Instituto Politécnico Nacional, México
28/08/2014–31/12/2016
Computational approach to aluminum biochemistry: al-phosphorylated polypeptide interactions.

Mauricio Rodriguez Mayorga
Universitat de Girona, Spain
01/12/2014–31/12/2017
Development of improved exchange-correlation functionals.

Grabiele Dalla Torre
Universita degli Studi di Milano, Italy
01/09/2015–30/04/2017
Theoretical chemistry.

Víctor Ramón Escobedo Bermúdez
Universidad de Salamanca, Spain
01/10/2015–30/09/2016
Literature and science.

Flavio Matias da Silva
Universidade Federal do Rio Grande do Sul, Porto Alegre, Brazil
15/10/2015–15/09/2016
Time dependent density functional theory applied to the interaction of charges and metallic media.

Prof. Raffaele Resta
Università di Trieste, Italy
02/12/2015–29/02/2016
Geometry and topology in electronic structure.

Prof. Juan Faustino Aguilera Granja
UASLP, Universidad Autónoma San Luis Potosí, México
10/12/2015–10/01/2016
Theoretical study of the electronic properties of transition metals on graphene sheet, and electronic properties of small binary clusters.

Dr. Natalia Cortés Muñoz
Universidad Técnica Federico Santamaria, Valparaiso, Chile
16/12/2015–15/06/2016
Electronic and thermal properties of two dimensional materials.

Prof. Giorgio Benedek
Universitá di Milano-Bicocca, Milano, Italy
11/01–28/02/2016
Surface phonons and phase transitions.

Dr. Angela Demetriadou
Imperial College London, UK
13/01–30/04/2016
Nanophotonics in ultranarrow gaps.

Prof. Gernot Frenking
Fachbereich Chemie, Philipps Universität Marburg, Marburg, Germany
01/02–31/03/2016
Theoretical chemistry.

Prof. Roman Kuzian
National Academy of Sciences of Ukraine, Kiev, Ukraine
01/02–30/04/2016
Photoemission from strongly correlated systems.

Diego Romero Abujetas
Instituto de Estructura de la Materia, IEM-CSIC
01/02–30/06/2016
Theory of light scattering in nano-structured highly refractive media.

Prof. Norman March
University of Antwerpen, Belgium
04/02–04/04/2016
Study of the role of exchange and correlation effects in both ground state density functional theory as well for excitation within time-dependent density-functional theory.

Prof. Joseph Richard Manson
Clemson University, South Carolina, USA
08/02–15/03/2016
Theoretical studies of structure and dynamics of microscopic surfaces.

Samuel Maciel Correa
Universidad Federal de Pará, Brazil
09/02–31/07/2016
Electron transport simulations of nanostructures.

Prof. Vladimir Nazarov
Research Center for Applied Sciences, Academia Sinica, Taipei, Taiwan
01/03–31/03/2016
Time-dependent density-functional theory of EELS of thin films on substrates.

Prof. Wolfgang Schattke
Institut für Theoretische Physik, Christian-Albrechts-Universität zu Kiel, Germany
01/03–31/05/2016
Quantum Monte-Carlo/Photoemission.

Prof. Victor Tugushev
National Research Center "Kurchatov Institute", Moscow, Russia
01/03–27/05/2016
Anomalous hall effect in topological insulators.

Prof. Valery Tyuterev
Tomsk State Pedagogical University, Tomsk, Russia
21/03–20/04/2016
Electron-phonon interaction in semiconductors and nanostructures.

Jorge Luis Hita
Universidad Autónoma de Madrid, Spain
28/03–28/06/2016
Theoretical analysis of optical binding induced by random field fluctuations.

Prof. Alexander Protogenov
Institute of Applied Physics of the Russian Academy of Sciences, Nizhnii Novgorod, Russia
04/04–03/05/2016
Interacting topological states on the surface of Dirac materials.

Dr. Mario Zapata Herrera
Universidad de los Andes, Bogotá, Colombia
04/04–30/06/2016
Quantum and classical approaches to the optical response of metallic nanostructures.

Thomas Lavoisier
Université Paris-Sud, France
25/04–25/07/2016
STM analysis of curved SrTiO3 surfaces.

Dr. Ziya Aliyev
Institute Catalysis and Inorganic Chemistry, Azerbaijan National Academy of Science, Baku, Azerbaijan
01/05–30/07/2016
Materials physics of topological insulators.

Prof. Francesca Ferlaino
Institut für Experimentalphysik, University of Innsbruck, Austria
30/05–22/08/2016
Quantum optics and quantum information.

Dr. Sergey Eremeev
Institute of Strength Physics and Materials Science, Tomsk, Russia
01/06–29/08/2016
Topological insulators.

Dr. Martin Horn
University of Konstanz, Germany
01/06–30/06/2016
Image segmentation using machine learning with ImageJ and KNIME.

Prof. Vladimir Menshov
National Research Centre "Kurchatov Institute", Moscow, Russia
01/06–30/08/2016
Electron properties and QAHE in magnetic topological insulator thin films.

Dr. Maria Corina Urdaniz Gonzalez
Comision Nacional de Energía Atómica, Buenos Aires, Argentina
05/06–12/08/2016
Magnetic properties of transition metal atoms on the CuCl surface.

Prof. Vladimir Nazarov
Research Center for Applied Sciences, Academia Sinica, Taipei, Taiwan
06/06–05/07/2016
Time-dependent density-functional theory of EELS of thin films on substrates.

Prof. Juan Faustino Aguilera Granja
UASLP, Universidad Autónoma San Luis Potosí, México
09/06–08/08/2016
Theoretical study of the electronic properties of transition metal on graphene.

Dr. Sara Barja Martinez
Max Planck Institute for Solid State Research, Stuttgart, Germany
15/06–03/11/2016
Electrochemistry of 2D transition metal dichalcogenides.

Dr. Tatiana Menshchikova
Tomsk State University, Russia
16/06–12/09/2016
Investigation of the electronic structure of topological insulators using first-principles calculations.

Dr. Igor Rusinov
Tomsk State University, Russia
16/06–12/09/2016
Investigation of materials for spintronics: topological semiconductors and bismuth tellurohalides.

Prof. Oleg Prezhdo
University of Southern California,
Los Angeles, California, USA
23/06–15/08/2016
Modeling of excitation dynamics in nanoscale materials using time-domain density functional theory and advanced techniques.

José Angel Castellanos Reyes
Universidad Autónoma Nacional de México, Mexico
29/06–05/08/2016
Induced forces by swift electrons on metallic nanoparticles.

Dr. Alejandro Reyes Coronado
Universidad Autónoma Nacional de México
29/06–05/08/2016
Induced forces by swift electrons on metallic nanoparticles.

Prof. Francisco José Garcia Vidal
Facultad de Ciencias, Universidad Autónoma de Madrid, Spain
01/07–31/08/2016
Quantum plasmonics.

Prof. Wlodzimierz Jaskólski
Nicolaus Copernicus University, Institute of Physics, Torun, Poland
01/07–31/07/2016
Topologically protected states in bilayer graphene.

Prof. Pavel Jelinek
Institute of Physics of the Czech Academy of Sciences Prague, Czech Republic
01/07–31/08/2016
Molecular nanostructures on surfaces.

Prof. Nikolay Kabachnik
Institut fur Experimentalphysik, Hamburg, Germany
01/07–30/09/2016
Study of Auger processes in gases and at solid surfaces within an attosecond streaking scheme.

Prof. Andrey Vasenko
Laboratoire de Physique et Modelisation des Milieux Condensed, CNRS, Grenoble, France
01/07–15/08/2016
Superconductor/ topological insulator proximity effect.

Prof. Jorge Kohanoff
Queen's University Belfast, Northern Ireland, UK
01/07–30/07/2016
Time-dependent density-functional theory for radiation damage

Dr. Fernando de Juan Sanz
IMDEA Nanociencia, Madrid
04/07–12/08/2016
Charge density waves in transition metal dichalcogenides and transport in HgTe quantum wells.

Prof. Carmen Mijangos Ugarte
Consejo Superior de Investigaciones Científicas, Instituto de Ciencia y Tecnología de Polímeros, Madrid, Spain
04/07–04/08/2016
Gradual polymer nanostructures by nanotemplating.

Prof. Luis Martin Moreno
Instituto de Ciencia de Materiales de Aragón, (ICMA), Zaragoza, Spain
07/07–06/08/2016
Nanophotonics.

Prof. Miguel Angel Cazalilla
National Tsing Hua University, Taiwan
11/07–11/08/2016
Spintronics of two dimensional materials.

Afaf El-Sayed Abdelmottaleb Masoud
Faculty of Science, Al-Azhar University, Cairo, Egypt
15/07–10/10/2016
Interactions at organic/metal interfaces measured by their adsorption heights.

Prof. Vladimir Kuznetsov
Tomsk State University, Tomsk, Russia
01/08–31/08/2016
Investigation of the electronic structure of topological insulators using first-principles calculations.

Prof. Gernot Frenking
Fachbereich Chemie, Philipps Universität Marburg, Germany
08/08–31/10/2016
Theoretical chemistry.

Yuri Hasegawa
University of Tsukuba, Japan
22/08.2016–15/02/2017
Self-assembled and covalently-coupled molecular networks on metallic surfaces.

Dr. Paul D. Bristowe
University of Cambridge, UK
01/09–30/09/2016
The properties of MAX phases from first principles.

Prof. Amand Lucas
University of Namur, Belgium
01/09–30/10/2016
Scattering of charged particles by surfaces.

José Manuel Guevara Vela
Universidad de Oviedo, Spain
04/09–04/12/2016
Intracules of the pair density in atoms and molecules.

Prof. Thomas A. Klar
Johannes Kepler University Linz,
Institute of Applied Physics, Linz, Austria
10/09–23/10/2016
Study of conduction properties in plasmonic junctions.

Prof. Giorgio Benedek
Universitá di Milano-Bicocca, Milano, Italy
11/09–31/10/2016
Surface phonons and phase transitions.

Dr. Leonor Chico Gomez
Instituto de Ciencia de Materiales de Madrid (ICMM), Spain
16/09–16/10/2016
Electronic and magnetic properties of graphene-based systems.

Prof. Joseph Richard Manson
Clemson University, South Carolina, USA
04/10–10/11/2016
Electron-phonon interactions at metal surfaces, and scattering of atoms and molecules from surfaces.

Prof. Julio A. Alonso Martín
Facultad de Ciencias, Universidad de Valladolid, Spain
01/11–30/11/2016
Interaction of molecules with metallic nanoparticles.

Prof. Talat Shahnaz Rahman
University of Central Florida, USA
01/12–01/02/2017
Surface coordination chemistry and development of many-body theories beyond DFT.

Short visits

Prof. Godfrey Gumbs
Hunter College, The City University of New York, USA
08/01–29/01/2016
Optical response properties of buckled 2D silicene.

Prof. Andreas Savin
Université Pierre et Marie Curie, Paris, France
11/01–22/01/2016
Adiabatic connection in DFT

Prof. Denis Vyalikh
Dresden University, Germany
13/01–23/01/2016
Photoemission measurements of magnetic surface states.

Prof. Christoph Geibel
MPI CPfS, Dresden, Germany
17/01–19/01/2016
Two hot topics related to quantum critical points: Fermi surface and charge density wave.

Prof. Cornelius Krellner
University of Frankfurt, Germany
21/01–23/01/2016
Correlated matter: Insights from new materials.

Dr. Pierre Fouché
CRPP, Centre de Rederche Paul Pascal
24/01–30/01/2016
Superradiance in plasmon-molecule hybrid systems.

Dr. James Beardmore
Keele University, Keele, UK
24/01–07/02/2016
Simulación teórica y caracterización del mecanismo de reacción de formación de hidroxialuminiosilicatos (HAS)

Dr. Pablo Aguado Puente
CIC nanoGUNE, Donostia / San Sebastián, Spain
01/02–14/02/2016
Coupling of ferroic nanoscale films with interfacial two dimensional electron gases in oxides.

Prof. Marijan Sunjic
University of Zagreb, Croatia
02/02–26/02/2016
Dynamical response and surface excitations in thin films.

Prof. Dimitri Batani
Université de Bordeaux, Talence, France
04/02–06/02/2016
Development of the PETAL laser facility and its applications in physics.

Prof. Marco Bernasconi
Department of Materials Science,
University of Milano-Bicocca, Italy
04/02–06/02/2016
Large Scale Simulations of Phase Change Materials for Data Storage.

Prof. Geert-Jan Kroes
Leiden Institute of Chemistry, Gorlaeus Laboratory, Leiden, Netherlands
07/02–05/03/2016
Electronic and surface temperature effects in the adsorption, desorption and scattering of diatomic molecules on metal surfaces

Anna Mandziak
Universidad Maria Curie-Sklodowska, Lublin, Poland
15/02–17/02/2016
Core-level investigations of curved crystals.

Kim Hanseul
Korea Advanced Institute of Science and Technology (KAIST), Republic of Korea
16/02–18/02/2016
Ab initio simulations of quantum transport.

Prof. Salvador Miret Artes
CSIC, Instituto de Física Fundamental, Madrid
23/02–27/02/2016
Theory of surface diffusion.

Prof. Sascha Husa
Universitat de les Illes Balears & Institut d'Estudis Espacials de Catalunya (IEEC), Spain
27/02–01/03/2016
Primer descubrimiento. Advanced LIGO.

Prof. Alicia Sintes Olives
Universitat de les Illes Balears & Institut d'Estudis Espacials de Catalunya (IEEC), Spain
27/02–01/03/2016
Primer descubrimiento. Advanced LIGO.

Dr. Andrea Donarini
Institute of Theoretical Physics,
University of Regensburg, Germany
28/02–01/03/2016
Transport characteristics of complex interacting nano-junctions.

Dr. Paula Abufager
Instituto de Física Rosario CONICET (Consejo Nacional de Investigaciones Científicas y Técnicas), Rosario, Argentina
05/03–02/04/2016
Inelastic effects on SAM.

Prof. Juan Faustino Aguilera Granja
UASLP, Universidad Autónoma San Luis Potosí, México
14/03–18/03/2016
Theoretical study of the electronic properties of transition metals on graphene sheet, and electronic properties of small binary clusters.

Dr. Jean Christophe Gimel
University of Angers, France
14/03/2018–18/03/2016
Diffusion of nanotracers in complex media.

Dr. Marta Prada
University of Hamburg, Germany
15/03–15/03/2016
Spintronics in low-dimensional heterostructures: a symmetry-based perspective.

Prof. Christian A. Nijhuis
National University of Singapore
20/03–22/03/2016
Electrical excitation, manipulation, and detection, of plasmons in molecular junctions.

Prof. Juan Faustino Aguilera Granja
UASLP, Universidad Autónoma San Luis Potosí, México
28/03–01/04/2016
Theoretical study of the electronic properties of transition metals on graphene sheet, and electronic properties of small binary clusters.

Prof. Friedrich Reinert
Universidad de Würzburg, Germany
30/03–03/04/2016
Electronic States in Topological insulators.

Dr. Helene Bouchiat
Laboratoire de Physique des Solides, Université Paris Sud, France
07/04–08/04/2016
Quantum interferences in bismuth nanowires based Josephson junctions: signature of topological ballistic edge states?

Prof. Roland Hayn
University d'Aix-Marseille, France
09/04–16/04/2016
Magnetic moment formation in metal-organic monolayers.

Prof. Rolf Heid
Karlsruhe Institute of Technology (KIT), Germany
10/04–13/04/2016
Electron phonon interaction in bulk metals and at surfaces.

Prof. Dieter Richter
IFF-FZ, Forschungszentrum Jülich, Germany
11/04–15/04/2016
Polymer dynamics by neutron techniques.

Dr. Michaela Zamponi
Forschungzentrum Julich, Germany
13/04–15/04/2016
Dynamics of branched polymers.

Prof. Ernesto Medina
Instituto Venezolano de Investigaciones Científicas, Caracas, Venezuela
14/04–18/04/2016
Spin orbit interaction in electron transport in chiral molecules.

Felix Benz
University of Cambridge, UK
18/04–22/04/2016
Single atom motion as a driver of vibrational pumping in an optical cavity.

Prof. Stefano Corni
Center S3, CNR Institute of Nanoscience, Modena, Italy
18/04–20/04/2016
An hybrid model for the optical properties of molecules close to plasmonic nanoparticles.

Dr. Andrey Borisov
Université Paris Sud, L'Institut des Sciences Moléculaires d'Orsay, France
20/04–30/04/2016
Quantum plasmonics.

Dr. Luis Rosales Ahumada
Universidad Técnica Federico Santa María, Chile
22/04–29/04/2016
Transport and thermoelectric properties of nano system.

Dr. Michele Burrello
Max Planck Institute of Quantum Optics, Garching, Germany
24/04–27/04/2016
Quantum engineering of non-Abelian phases of matter.

Prof. Barbara Kraus
Universität Innsbruck & IQOQI, Inssbruck, Austria
09/05–13/05/2016
Entanglement and LU/LOCC classification of fermionic Gaussian states.

Cornelia Spee
Universität Innsbruck & IQOQI, Austria
09/05–13/05/2016
Entanglement and LU/LOCC classification of fermionic Gaussian states.

Prof. Justin Wells
Norwegian University of Science and Technology (NTNU), Trondheim, Norway
10/05–14/05/2016
Electron-phonon interactions in graphene.

Prof. Thiagarajan Balasubramanian
MAX IV Laboratory, Lund University, Sweden
11/05–13/05/2016
Electron-phonon interactions in graphene.

Prof. Bo Hellsing
Gothenburg University, Sweden
11/05–14/05/2016
Electron-phonon interactions in graphene.

Dr. Laurent Limot
CNRS, Strasbourg, France
11/05–13/05/2016
Molecular spintronics using single metallocenes.

Dr. Federico Mazzola
Norwegian University of Science and Technology (NTNU), Trondheim, Norway
12/05–13/05/2016
Photoemission spectroscopies and their application in solid state and material physics.

Prof. Yutaka Wakayama
National Institute for Materials Science (NIMS), Tsukuba, Ibaraki, Japan
12/05–17/05/2016
Molecular assemblies on metal surfaces.

Dr. Sara Capponi
Cardiovascular Research Institute, University of California in San Francisco, USA
15/05–22/05/2016
Nanoconfined water in a channel-like protein.

Prof. Simone Napolitano
Université Libre de Bruxelles (ULB) Laboratory of Polymer and Soft Matter Dynamics, Faculté des Sciences, Belgium
16/05–18/05/2016
Polymer dynamics in confinement.

Dr. Daniel Wegner
Radboud University, Institute for Molecules and Materials, Nijmegen, Netherlands
18/05–20/05/2016
Finding and tuning electronic "set screws" in molecular magnets and phosphorescent complexes.

Dr. Nicolas Large
Northwestern University, Chicago, USA
19/05–21/05/2016
Optical response in plasmonic nanostructures.

Prof. Amy Catanzano
Wake Forest University, North Carolina, USA
23/05–25/05/2016
Quantum poetics: language and reality in physics and poetry.

Prof. Franz Himpsel
University of Wisconsin, Madison, USA
28/05–08/06/2016
Electronic states of organic molecules for solar cells.

Prof. Peter Saalfrank
Institut für Chemie, Universität Postdam, Postdam-Golm, Germany
28/05–03/06/2016
Elastic, inelastic, and reactive scattering of atoms and molecules from surfaces.

Dr. Ferran Feixas
Universitat de Girona, Spain
31/05–05/06/2016
Accelerated molecular dynamics: a versatile tool to study protein dynamics, protein folding and biomolecular recognition.

Prof. Juan Luis Suarez
CulturePlex Lab at Western University, Ontario, Canada
06/06–08/06/2016
Cultural Analytics. The Humanistic Science of Culture.

Dr. Daijiro Nozaki
University of Paderborn, Germany
08/06–11/06/2016
Interference phenomena in open quantum systems: applications for molecular switches and thermo-electric devices.

Tobia Mancabelli
Ludwig-Maximilians-Universität, Munich, Germany
12/06–18/06/2016
Study of quantum effects in Raman scattering of graphene samples.

Prof. Ceferino López
Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Spain
13/06–16/06/2016
Light scattering in random media.

Prof. Eugene Kogan
Bar-Ilan University, Ramat-Gan, Israel
16/06–30/06/2016
Critical phenomena in disorder magnets.

Prof. Wolfgang Paul
Institut für Physik, Martin Luther University Halle-Wittenberg, Germany
17/06–23/06/2016
Relaxation processes and glass transition of confined 1,4-polybutadiene.

Dr. Remi Avriller
CNRS Laboratoire Ondes et Matière d'Aquitaine (LOMA) Université de Bordeaux et CNRS, Talence, France
20/06–24/06/2016
Quantum transport and nanoelectromechanical systems.

Dr. Martin Zeppenfeld
Max-Planck Institut fuer Quantenoptik (MPQ), Garching, Germany
22/06–25/06/2016
Trapping and manipulating cold polar molecules. Electronic states of organic molecules for solar cells.

Prof. David Johnson
University of Oregon, USA
22/06–24/06/2016
Syntesis of two D materials.

Prof. Vladimir Chaldyshev
Ioffe Physico-Technical Institute Russian Academy of Science, St. Petersburg, Russia
25/06–02/07/2016
Plasmonic properties of metal nanoparticles in semi-conducting materials.

Prof. Andres Diaz Gil
Instituto de Física Teórica (UAM-CSIC), Madrid, Spain
26/06–29/06/2016
Software carpentry: best practices for scientific computing.

Prof. Geert-Jan Kroes
Leiden Institute of Chemistry, Gorlaeus Laboratory, Leiden, Netherlands
26/06–09/07/2016
Electronic and surface temperature effects in the adsorption, desorption and scattering of diatomic molecules on metal surfaces.

Prof. Gabriel Molina Terriza
Macquarie University, Sydney, Australia
26/06–15/07/2016
Enhancing circular dichroism with dual nanostructures.

Prof. Ravindra Chhajlany
Faculty of Physics, Adam Mickiewicz University, Poznan, Poland
27/06–03/07/2016
Non-standard Hubbard model in optical lattices.

Prof. Andrei Borisov
Université Paris Sud, France
03/07–31/07/2016
Quantum plasmonics

Prof. Francisco Guinea López
IMDEA Nanoscience, Madrid, Spain
03/07–31/07/2016
Two dimensional materials.

Prof. Maria Angeles Hernandez Vozmediano
Instituto de Ciencia de Materiales de Madrid, Consejo Superior de Investigaciones Científicas, CSIC, Madrid, Spain
03/07–30/07/2016
Analysis of interactions, disorder, and lattice distortions in topological insulators and graphene.

Dr. Pascal Larregaray
Institut des Sciences Moléculaires, Université de Bordeaux, France
04/07–27/07/2016
Ab-initio methods for studying the physics and chemistry of adsorption processes at surfaces.

Dr. Hendrik Bentmann
University of Würzburg, Germany
05/07–07/07/2016
Photoelectron spectroscopy study of spin-orbit interaction at surfaces.

Prof. Leonid Glazman
Yale University, Connecticut, USA
10/07–30/07/2016
Spin-dependent transport in low dimensional semiconducting structures.

Dr. Jerome Cayssol
Université Bordeaux, LOMA, France
11/07–12/07/2016
Quantum transport in excitonic condensates

Prof. Manuel Nieto Vesperinas
Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Spain
11/07–15/07/2016
Theory of optical torques on small particles.

Prof. Giovanni Vignale
University of Missouri-Columbia, Columbia, USA
16/07–24/07/2016
Condensed matter theory.

Prof. Albert Fert
UMR CNRS Thales, Palaiseau, France
17/07–21/07/2016
Conversion between spin and charge currents at room temperature by Rashba or Topological Insulato interfaces and perspective for low power spintronic devices.

Dr. Cosimo Gorini
Universität Regensburg, Regensburg, Germany
17/07–22/07/2016
Dissipative transport in systems with flat bands.

Prof. Angela Camacho
Universidad de los Andes, Bogotá, Colombia
18/07–19/07/2016
Nanosecurity: a Colombian initiative.

Prof. Ulrich Höfer
PhilippsUniversität Marburg, Germany
20/07–27/07/2016
Resonance hopping on surfaces of simple metals.

Prof. Alexander Golubov
University of Twente, Netherlands
31/07–07/08/2016
Topological superconductivity.

Prof. Garnett Bryant
NIST, Gaithersburg, Maryland, USA
21/08–30/08/2016
Nanophotonics.

Prof. Bogdan Andrei Bernevig
Princeton University, New Jersey, USA
22/08–08/09/2016
Topological insulators.

Dr. Zhijun Wang
Princeton University, NJ, United States
22/08–11/09/2016
Topologically ordered phases of matter.

José Daniel Mella Riquelme
Universidad de Chile, Santiago, Chile
26/08–11/09/2016
Topological crystalline insulator

Dr. Thomas Hendel
Institute of Chemistry of Humboldt-University of Berlin, Germany
29/08–05/09/2016
Photonics of hybryd structures.

Prof. Archie Howie
Cavendish Laboratory, University of Cambridge, Cambridge, UK
05/09–19/09/2016
Electron energy loss and decoherence.

Prof. Harald Brune
Institute of Physics, EPFL, Switzerland
07/09–09/09/2016
Realizing the smallest surface adsorbed quantum magnets.

Dr. Elias Diesen
Stockholm University, Sweden
11/09–16/09/2016
Vibrational effects in resonant X-ray emission.

Iurii Zhovtobriukh
Stockholm University, Sweden
11/09–16/09/2016
Vibrational effects in resonant X-ray emission.

Dr. Akshay Rao
Cavendish Laboratory, University of Cambridge, UK
13/09–14/09/2016
Singlet exciton fission: a path to break the shockley-queisser limit on the efficiency of photovoltaics.

Prof. Teheodore Einstein
University of Maryland, United States
14/09–18/09/2016
Elastic Interactions between surface steps.

Prof. Yutaka Wakayama
National Institute for Materials Science (NIMS), Tsukuba, Ibaraki, Japan
20/09–01/10/2016
Molecular assemblies on metal surfaces.

Prof. Archie Howie
Cavendish Laboratory, Cambridge, UK
26/09–03/10/2016
Electron energy loss and decoherence. Participate in Passion for Knowledge Meeting.

Dr. Jean Christophe Tremblay
Freie Universität Berlin, Germany
26/09–30/09/2016
Simulation of STM-induced tautomerization within a single porphycene molecule on Cu(111)

Prof. Marijan Sunjic
University of Zagreb, Croatia
03/10–30/10/2016
Dynamical response and surface excitations in thin films.

Prof. Salvador Miret Artes
CSIC, Instituto de Física Fundamental, Madrid, Spain
23/10–26/10/2016
Theory of surface diffusion.

Dr. Andreas Schnyder
Max Planck Institute for Solid State Research, Stuttgart, Germany
26/10–28/10/2016
Design and characterization of new topological materials.

Dr. Leslie Schoop
Max Planck Institute for Solid State Research, Stuttgart, Germany
26/10–30/10/2016
New fermions.

Prof. Dimitri Batani
Université de Bordeaux, Talence, France
27/10–30/10/2016
Development of the PETAL laser facility and its applications in physics.

Dr. Donaldi Mancelli
Université de Bordeaux, Talence, France
27/10–28/10/2016
Development of the PETAL laser facility and its applications in physics.

Prof. Denis Vyalikh
Dresden University, Germany
30/10–03/11/2016
Photoemission measurements of magnetic surface states.

Dr. Alexander Fedorov
Universität Köln and IFW Dresden, Germany and St. Petersburg State University, Russia
31/10–03/11/2016
Electronic properties of doped graphene and graphene nanoribbons: photoemission study.

Yael Gutierrez Vela
Universidad de Cantabria, Santander, Spain
02/11–30/11/2016
Calculation of optical constants from ab initio calculations.

Dr. Barry Bradlyn
Princeton University, USA
12/11–19/11/2016
Topological quantum chemistry.

Prof. Mikael Kepenekian
CNRS, Institut des Sciences Chimiques de Rennes, Université de Rennes 1, France
14/11–25/11/2016
Spin-orbit electron transport from first principles.

Dr. Laura Fernandez Gomez-Recuero
Philipps University of Marburg, Germany
15/11–01/12/2016
Doped-graphene for electrochemical energy storage.

Prof. Tadaaki Nagao
National Institute of Materials Science, Tsukuba, Japan
22/11–30/11/2016
Wavelength selective perfect absorbers for infrared devices.

Dr. Ming Hao Liu
University of Ratisbona, Germany
23/11–29/11/2016
Quantum transport in system with bosonic conical intersection.

Prof. Shuichi Murakami
Tokyo Institute of Technology, Japan
23/11–26/11/2016
Physics of topological insulators and topological semimetals.

Prof. Motoaki Hirayama
Tokyo Institute of Technology, Japan
23/11–26/11/2016
Physics of topological insulators and topological semimetals.

Prof. Arno Rauschenbeutel
Institute of Atomic and Subatomic Physics, Vienna University of Technology, Austria
23/11–25/11/2016
Nanofiber-based atom light quantum interfaces.

Prof. Sang Hyun Oh
University of Minnesota, Minneapolis, USA
24/11–29/11/2016
Nanoplasmonics.

Prof. Pier A. Mello
Instituto de Física, Universidad Nacional Autónoma de México, (UNAM) D.F., Mexico
26/11–11/12/2016
Transport through disordered conductors and waveguides.

Fernando Izquierdo Ruiz
Universidad de Oviedo, Spain
27/11–03/12/2016
Calculation of anharmonic modes in clathrate hydrates.

Prof. José Manuel Recio
Universidad de Oviedo, Spain
27/11–28/11/2016
Calculation of anharmonic modes in clathrate hydrates.

Dr. Christian Pedersen
DTU, Technical University of Denmark, Denmark
28/11–23/12/2016
Transport properties of graphenic nanostructures.

Prof. Andrey Borissov
Université Paris Sud, France
08/12–10/12/2016
Quantum plasmonics.

Dr. Lukas Gallmann
Institute of Quantum Electronics, ETH Zürich, Switzerland
08/12–09/12/2016
Attophysics.

Prof. Ursula Keller
Institute of Quantum Electronics, ETH Zürich, Switzerland
08/12–09/12/2016
Attophysics.

Dr. Matteo Lucchini
Institute of Quantum Electronics, ETH Zürich, Switzerland
08/12–09/12/2016
Attophysics.

Prof. Anastassia N. Alexandrova
University of California, Los Angeles, USA
13/12–21/12/2016
Quantum chemistry and chemical bonding of small catalytic clusters.

Dr. Mikolaj Kajetan Schmidt
Faculty of Physics, Warsaw University, Poland
13/12–17/12/2016
Two-photon frequency-resolved correlations in optomechanical systems.

Prof. Rémi Carminati
Institut Langevin, ESCPI ParisTech, France
18/12–22/12/2016
Near field effects and multiple scattering of light.

Personnel

Administration

Ana López de Goicoechea
Administrator

Amaia Etxaburu
President's Assistant

María del Mar Álvarez
Secretary

Nerea Fariñas
Secretary

Karmela Alonso
Secretary

Beatriz Suescun
Acquisition of Scientific and
Management Equipment Technician

Outreach

Nora Gonzalez
Outreach Manager

Amaia Arregi
Outreach Officer

Computing Center

Txomin Romero
Computing Center Director

Belén Isla
Computing Center Assistant Director and
HPC Systems Manager

Carmen Martín
Systems, Security and Networks Manager

Luz Fernández
Operation and Help Desk Manager

Diego Lasa
Computing Services Manager

Daniel Franco
HPC Resources Technician

Seminars

1 **Why are insulators insulating?**
Prof. Raffaele Resta
Università di Trieste, Trieste, Italy
15/01/2016

2 **Two hot topics related to quantum critical points: Fermi surface and charge density wave**
Prof. Christoph Geibel
MPI CPfS, Dresden, Germany
18/01/2016

3 **Correlated matter: insights from new materials**
Prof. Cornelius Krellner
Goethe University Frankfurt, Germany
22/01/2016

4 **Large scale simulations of Phase change materials for data storage**
Prof. Marco Bernasconi
University of Milano-Bicocca, Milano, Italy
05/02/2016

5 **Many-body correlations in a Cu-phthalocyanine STM single molecule junction**
Dr. Andrea Donarini
Institute of Theoretical Physics, University of Regensburg, Germany
29/02/2016

6 Spintronics in low-dimensional heterostructures: a symmetry-based perspective
Dr. Marta Prada
Department of Physics, Universität Hamburg, Germany
15/03/2016

7 Diffusion of nanotracers in complex media
Dr. Jean Christophe Gimel
University of Angers, France
16/03/2016

8 Electrical excitation, manipulation, and detection, of plasmons in molecular junctions
Prof. Christian A. Nijhuis
National University of Singapore
21/03/2016

9 Exploring the photoemission intensity in ARPES: information beyond band structure
Prof. Friedrich Reinert
University of Würzburg, Germany
01/04/2016

10 Quantum interferences in bismuth nanowires based Josephson junctions: signature of topological ballistic edge states?
Dr. Helene Bouchiat
Laboratoire de Physique des Solides, Université Paris Sud, France
08/04/2016

11 Magnetic moment formation in metal-organic monolayers
Dr. Roland Hayn
Aix Marseille Université, France
12/04/2016

12 Spin orbit interaction in electron transport in chiral molecules
Prof. Ernesto Medina
Instituto Venezolano de Investigaciones Científicas, Caracas, Venezuela
15/04/2016

13 An hybrid model for the optical properties of molecules close to plasmonic nanoparticles
Prof. Stefano Corni
Center S3, CNR Institute of Nanoscience, Modena, Italy
19/04/2016

14 Weyl semimetals with synthetic gauge potentials
Dr. Michele Burrello
Max Planck Institute of Quantum Optics, Garching, Germany
25/04/2016

15 Photoemission spectroscopies and their application in solid state and material physics
Dr. Federico Mazzola
Norwegian University of Science and Technology (NTNU), Trondheim, Norway
12/05/2016

16 Molecular spintronics using single metallocenes
Dr. Laurent Limot
Institut de Physique et de Chimie des Matériaux de Strasbourg CNRS, France
13/05/2016

17 Nanoconfined water in a channel-like protein
Dr. Sara Capponi
Cardiovascular Research Institute, University of California in San Francisco, San Francisco, USA
17/05/2016

18 Analysis of dielectric spectra beyond the relaxation time.
What can we learn from the dielectric strength?
Prof. Simone Napolitano
Université Libre de Bruxelles (ULB) and Laboratory of Polymer and Soft Matter Dynamics, Faculté des Sciences, Belgique
17/05/2016

19 Finding and tuning electronic "set screws" in molecular magnets and phosphorescent complexes
Dr. Daniel Wegner
Radbout Universiteit Nijmegen, Institute for Molecules and Materials, Nijmegen, Netherlands
19/05/2016

20 Quantum poetics: language and reality in physics and poetry.
Prof. Amy Catanzano
Wake Forest University in North Carolina, Winston Salem, USA
25/05/2016

21 Dynamics in photoexcited molecules: from photophysics to photochemistry.
Prof. Peter Saalfrank
Institut für Chemie, Universität Postdam, Postdam-Golm, Germany
02/06/2016

22 Accelerated molecular dynamics: a versatile tool to study protein dynamics, protein folding and biomolecular recognition.
Dr. Ferran Feixas
Universitat de Girona, Spain
03/06/2016

23 Cultural analytics. The humanistic science of culture
Prof. Juan Luis Suarez Sanchez de León
CulturePlex Lab at Western University, Ontario, Canada
07/06/2016

24 Interference phenomena in open quantum systems:
Applications for molecular switches and thermoelectric devices
Dr. Daijiro Nozaki
University of Paderborn, Germany
09/06/2016

25 Relaxation processes and glass transition of confined 1,4-polybutadiene
Prof. Wolfgang Paul
Institut für Physik, Martin Luther Universität Halle-Wittenberg, Germany
21/06/2016

26 Controlled molecular ensembles at cold and ultracold temperatures
Dr. Martin Zeppenfeld
Max-Planck Institut fuer Quantenoptik (MPQ), Garching, Germany
24/06/2016

27 Spin-orbit interaction in the electronic structure of surfaces and its detection by photoelectron spectroscopy
Dr. Hendrik Bentmann
University of Würzburg, Germany
06/07/2016

28 Even nanoparticles get the entanglement
Prof. Gabriel Molina Terriza
Macquarie University, Sydney, Australia
07/07/2016

29 Physics in Colombia is in its forties
Prof. Angela Camacho
Universidad de los Andes, Bogotá, Colombia
08/07/2016

30 Quantum dots artificial atoms, large molecules or small pieces of bulk?
Insights from time-domain Ab initio studies
Prof. Oleg Prezhdo
University of Southern California, Los Angeles, California, USA
15/07/2016

31 Photogalvanic effects in 2D materials and Weyl semimetals
Dr. Fernando de Juan Sanz
IMDEA Nanociencia, Madrid, Spain
26/07/2016

32 DNA radiation damage: insights from ab initio molecular dynamics simulations
Prof. Jorge Kohanoff
Atomistic Simulation Centre, School of Mathematics and Physics, Queen's University Belfast,
Northern Ireland, UK
27/07/2016

33 Realizing the smallest surface adsorbed quantum magnets
Prof. Harald Brune
Institute of Physics, EPFL, Switzerland
08/09/2016

34 Singlet exciton fission: A path to break the shockley-queisser limit on the efficiency of photovoltaics
Dr. Akshay Rao
Cavendish Laboratory, University of Cambridge, UK
13/09/2016

35 Physics of stepped surfaces: spinless fermions and beyond
Prof. Theodore Einstein
University of Maryland, USA
15/09/2016

36 Modelling of hybrid organic-inorganic materials
Prof. Paul D. Bristowe
University of Cambridge, Cambridge, UK
23/09/2016

37 Plasmonic nanoparticles and fluorescence
Prof. Thomas A. Klar
Institute of Applied Physics, Johannes Kepler University Linz, Austria
28/09/2016

38 Three-dimensional topological Dirac materials
Dr. Andreas Schnyder
Max Planck Institute for Solid State Research, Stuttgart, Germany
27/10/2016

39 Dirac materials from a chemist's perspective
Dr. Leslie Schoop
Max Planck Institute for Solid State Research, Stuttgart, Germany
27/10/2016

40 In search of the strongest steel: atomistics for daily life
Prof. Javier Gil Sevillano
TECNUN, Universidad de Navarra, Donostia / San Sebastián, Spain
28/10/2016

41 Electronic properties of doped graphene and graphene nanoribbons: photoemission study
Dr. Alexander Fedorov
Universität zu Köln and IFW Dresden, Germany and St Petersburg State University, Russia
02/11/2016

42 Topological quantum chemistry
Dr. Barry Bradlyn
Princeton University, New Jersey, USA
17/11/2016

43 Wavelength selective perfect absorbers for infrared devices
Prof. Tadaaki Nagao
National Institute of Materials Science, Tsukuba, Japan
23/11/2016

44 Nanofiber photonics and quantum optics
Prof. Arno Rauschenbeutel
Institute of Atomic and Subatomic Physics, Vienna University of Technology, Austria
24/11/2016

45 Electron optics in ballistic graphene
Dr. Ming-Hao Liu
Institut fuer Theoretische Physik, Universitaet Regensburg, Germany
25/11/2016

46 Interplay between topology and symmetry in topological semimetals
Prof. Shuichi Murakami
Tokyo Institute of Technology, Tokyo, Japan
25/11/2016

47 Ultra-flat and ultra-small: towards atomic-resolution engineering of metallic nanostructures
Prof. Sang Hyun Oh
University of Minnesota, USA
28/11/2016

48 Statistical scattering of waves: from the atomic nucleus to mesoscopic systems to disordered waveguides: an overview of past and new results
Prof. Pier A. Mello
Instituto de Física, Universidad Nacional Autónoma de México, (UNAM), México
29/11/2016

49 Transport Through Disordered Conductors and Waveguides: The Density Inside the Sample. A Maximum-Entropy Approach
Prof. Pier A. Mello
Instituto de Física, Universidad Nacional Autónoma de México, (UNAM) D.F., Mexico
02/12/2016

50 Attophysics in solids
Prof. Ursula Keller (ETH Zurich)
Institute of Quantum Electronics, ETH Zürich, Switzerland
09/12/2016

51 Boron in Functional Materials: from clusters and catalytic surfaces to ultra-hard alloys
Prof. Anastassia N. Alexandrova
University of California, Los Angeles, USA
15/12/2016

Workshops

Responsible Research and Innovation (RRI): The Problematic Quest for "Right" Impacts

March 10-11, 2016
DIPC, Donostia / San Sebastián

Organizing Committee
Patricio Carezzana (Universidad Nacional Autónoma de México)
Andoni Eizagirre (Mondragon University)
Erik Fisher (CSPO – Arizona State University)
Javier García Fronti (Universidad de Buenos Aires)
Margoth González (UPV/EHU)
Andoni Ibarra (UPV/EHU)
Hannot Rodríguez (UPV/EHU)

Scientific Committee
Ellen-Marie Forsberg (Oslo and Akershus University College)
Armin Grunwald (Institute for Technology Assessment and Systems Analysis at Karlsruhe Institute of Technology)
Andoni Ibarra (UPV/EHU)
Carl Mitcham (Colorado School of Mines)
Daniel Sarewitz (CSPO – Arizona State University)
Roger Strand (University of Bergen)

Invited Speakers
Marian Deblonde (Flemish Institute for Technological Research)
Andoni Eizagirre (Mondragon University)
Erik Fisher (CSPO – Arizona State University)
Ellen-Marie Forsberg (Oslo and Akershus University College)
David Guston (CSPO – Arizona State University)
Andoni Ibarra (UPV/EHU)
Hannot Rodríguez (UPV/EHU)
Jack Spaapen (Royal Netherlands Academy of Arts and Sciences)
René von Schomberg (European Commission, Brussels)
Brian Wynne (Lancaster University)
Clare Shelley-Egan (Oslo and Akershus University)
Phil Macnaghten (Wageningen University)
Sujatha Raman (University of Nottingham)
Sophie Pellé (University of Paris 1)
Arie Rip (University of Twente)
Stevienna de Saille (University of Sheffield)
Fabien Medvecky (University of Otago)
Andrea Saltelli (University of Bergen, and Autonomous University of Barcelona)
Mario Giampietro (Autonomous University of Barcelona, and Catalan Institution for Research and Advanced Studies)

The European Commission claims that research and engineering activities under the next R&D Framework Programme, "Horizon 2020" (2014-2020), will be conducted according to a "Responsible Research and Innovation" (RRI) framework, meaning that "societal actors work together during the whole research and innovation process in order to better align both the process and its outcomes, with the values, needs and expectations of European society" (EC, 2012, p. ii). RRI can be understood thus as an effort to justify innovation not on grounds of uncritical, or taken for granted macro-economic assumptions, but on the basis of societally-beneficial objectives, or challenges, as openly defined and debated by a plurality of societal actors. As such, RRI-based EU policy aims to introduce "broader foresight and impact assessments for new technologies, beyond their anticipated market-benefits and risks" (von Schomberg 2013, p. 51).

Explicitly characterized as a "challenge-based approach", Horizon 2020 claims therefore to be prepared and oriented to address"major concerns shared by citizens in Europe and elsewhere", including human and environmental health, sustainability, energy efficiency, climate action, inclusiveness, security, and freedom.[1] However, are these generic challenges self-evident? How are they constituted and by whom? Can those challenges be challenged? How are they operationalized? On what normative bases? These and other similar questions express a legitimate concern for the main dynamics, assumptions and priorities by which normative frameworks are constituted and institutionalized in RRI-based EU research policy. This conference aimed to interrogate the heterogeneous and contingent socio-technical processes that guide, enable and also constrain RRI's quest for "right" impacts.

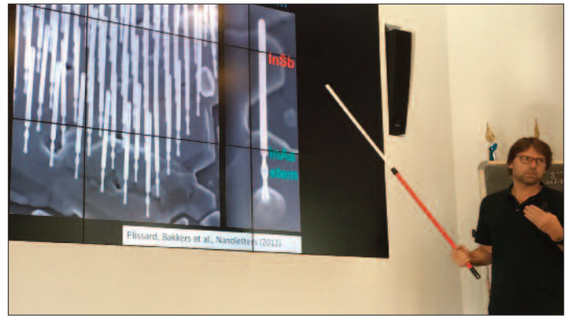
12th Capri Spring School on Transport in Nanostructures 2016

April 11-15, 2016
Villa Orlandi, Isola di Capri, Italy
http://www.capri-school.eu/capri16/

Organizing Committee
Dario Bercioux (Ikerbasque, DIPC)
Alessandro De Martino (City University London)
Reinhold Egger (Heinrich-Heine-Universität - Düsseldorf)
Hermann Grabert (Albert-Ludwig-Universität - Freiburg)
Christian Schönenberger (Universität Basel)
Arturo Tagliacozzo (Università "Federico II" Napoli)

This one week school provided several three to four hour lectures by leading experts supplemented by a few shorter seminars. As usual, the conference venue was Centro Multimediale "Mario Cacace" of Comune di Anacapri, and accommodation was provided in nearby hotels. While the school is primarily aimed at instructing PhD students and young postdoctoral researchers, more senior scientists who want to acquaint themselves with the subject of the school were also welcome.

Invited Speakers
Yaroslav Blanter (Delft)
Christoph Bruder (Basel)
Yuval Gefen (Weizmann)
Steve Girvin (Yale)
Leo Kouwenhoven (Delft)
Jukka Pekola (Aalto)
Jason Petta (Princeton)



Towards Reality in Modelling of Molecular Electronics

June 13-17, 2016
Miramar Palace, Donostia / San Sebastián
http://trmme.dipc.org/

Organizing Committee
Daniel Sanchez-Portal (CFM (CSIC-UPV/EHU), DIPC)
Adam Foster (Aalto University)
Pedro Brandimarte (UPV/EHU)
Mads Engelund (UPV/EHU)
Thomas Frederiksen (Ikerbasque, DIPC)
Aran Garcia Lekue (Ikerbasque, DIPC)
Karmela Alonso Arreche (DIPC)

Donostia International Physics Center (DIPC) and FET-ICT project Planar Atomic and Molecular Scale devices (PAMS) organized the international workshop Towards Reality in Modelling of Molecular Electronics (TRMME) that took place in Donostia / San Sebastián, Spain, on June 13-17, 2016.

The aim of this workshop was to bring together experienced and young researchers, as well as students, working in the field of the theory of quantum transport and the development of computational tools for transport simulations in the nanoscale.

Invited Speakers
Fernando Delgado, CFM CSIC-UPV/EHU, San Sebastian, Spain
Andrea Donarini, Universität Regensburg, Germany
Jaime Ferrer, Universidad de Oviedo, Spain
Rafael Gutierrez, TU Dresden, Germany
Antti-Pekka Jauho, DTU Nanotech, Denmark
Yong-Hoon Kim, KAIST, Korea
Stefan Kurth, Univ. del País Vasco UPV/EHU, Spain
Colin J. Lambert, Lancaster University, UK
Alejandro Lopez-Bezanilla, Argonne National Laboratory, USA
Vincent Meunier, Rensselaer Polytechnic Institute, USA
Branislav K. Nikolić, University of Delaware, USA
Nick R. Papior, DTU Nanotech, Denmark
Fabian Pauly, University of Konstanz, Germany
Alessandro Pecchia, CNR-ISMN Rome, Italy
Uri Peskin, Technion, Israel
Alexandre R. Rocha, Univ. Est. Paulista, São Paulo, Brazil
Stephan Roche, ICN2 Barcelona, Spain
Dvira Segal, University of Toronto, Canada
Kurt Stokbro, QuantumWise A/S, Denmark
Michael Thoss, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany
Massimiliano Di Ventra, University of California San Diego, USA
Jian-Sheng Wang, National University of Singapore

Basque Quantum Science and Technologies Workshop

June 14, 2016
CIC nanoGUNE, Donostia / San Sebastián

Organizing Committee
Geza Giedke (Ikerbasque, DIPC)
Lucas Lamata (UPV/EHU Bilbao)
Nacho Pascual (Ikerbasque, CIC nanoGUNE)

The aim of this workshop was to bring together researchers based in the Basque Country who are working or are interested in starting to work on quantum science and technology to discover or explore joint interests and to discuss and evaluate the prospects of some joint effort in view of the recently announced flagship initiative.

Invited speakers
Nacho Pascual (CIC nanoGUNE)
Gonzalo Muga (UPV/EHU Bilbao)
Javier Aizpurua (CFM (CSIC-UPV/EHU), DIPC)
Vitaly Golovach (CFM (CSIC-UPV/EHU), DIPC)
Enrique Solano (UPV/EHU Bilbao)
Géza Tóth (UPV/EHU Bilbao)
Geza Giedke (Ikerbasque, DIPC)

Special Session

Social and Scientific-Technical Knowledge at the Service of Sustainable Human Development

June 15, 2016
DIPC, Donostia / San Sebastián

Social and scientific-technical knowledge at the service of Sustainable Human Development was organized by Agirre Lehendakaria Center for Social and Political Studies (ALC) in partnership with the Provincial Council of Gipuzkoa and the Donostia International Physics Center (DIPC),

During the last three years ALC has been developing several research projects based on the Basque experience around Sustainable Human Development from a multidisciplinary approach that included society, economy, environment and Human Rights.

The outcome of this research work was discussed. The key to understanding what the Basque Country has achieved so far – as well as to construct its own future – lies in the influence that cultural aspects had on the main strategic decisions taken, both in public and private spheres. During the seminar the potential of this "K" to guide our future was discussed.

Contributions

Introduction
Markel Olano, General Deputy of Gipuzkoa

"The two cultures"
Pedro Miguel Etxenike, president of DIPC

"The K is the Key" **Juan José Ibarretxe**, director of Agirre Lehendakaria Center, University of the Basque Country (UPV/EHU), former President of the Basque Country

"SHD: Empirical modeling work"
Joshua Fisher, Columbia University

"SHD. Sustainable peace"
Peter Coleman, Columbia University

"A citizen science research project"
Armando Geller, Basque Peace Process Scenarios.

"Sustainable Human Development"
Andrea Bartoli, School of Diplomacy and International Relations, Seton Hall University

iPolymorphs. Novel Routes to Inorganic Polymorphs

June 22-24, 2016
Materials Physics Center (CFM), Donostia / San Sebastián
http://ipolymorphs.dipc.org/

Organizing Committee
Stefan Bromley (Universitat de Barcelona)
Jon M. Matxain (UPV/EHU and DIPC)

Polymorphism is the capacity of a solid material to exist in more than one crystal structure (where here we take this definition to include elemental polymorphism, or allotropy). Often changes in crystal structure can lead to new properties and the opening up of the range of potential applications of a single compound (e.g. two different polymorphs of BN can be used an an abrasive or a lubricant respectively). The number of naturally occurring metastable polymorphs for any one inorganic compound is relatively scarce and typically amounts to a handful of crystal structures at most. Synthesis of metastable inorganic polymorphs is also difficult, due the high temperatures typically employed in solid state inorganic synthesis which tends to produce the most thermodynamically stable crystal structure. High-pressure techniques provide a means to obtain new dense polymorphs, which are, however, often difficult to quench to ambient conditions.

Over the last few decades numerous theoretical predictions and new experimental synthesis (e.g. low temperature deposition, novel templating methods, degassing of high pressure phases) have begun to expand the world of novel metastable polymorphs. Often the collaboration of both theoreticians and experimentalists has been crucial for these advances. This workshop intended to further encourage a productive cross fertilization of predictive theory and new experimental methods, providing a space for exchange and creation of new ideas.

Plenary Speakers
Prof. Timothy A. Strobel, Geophysical Laboratory, Carnegie Institution of Science, Washington, USA
Prof. Dr. Richard Dronskowski, Chair of Solid-State and Quantum Chemistry, RWTH Aachen, Germany
Prof. C. Richard A. Catlow, Materials and Inorganic Chemistry, University College London, London, UK
Prof. Matthias Scheffler, Theory Department, Fritz Haber Institute of the Max Planck Society, Germany
Dr. John Claridge, Chemistry Department, University of Liverpool, Liverpool, UK

Keynote Speakers
Dr. Ion Errea, Department of Applied Physics, University of the Basque Country (UPV/EHU) and DIPC associate
Prof. Wojciech Grochala, University of Warsaw, Poland
Prof. Christian Schoen, Max Planck Institute for Solid State Research, Germany
Prof. Davide M. Proserpio, Universita degli Studi di Milano, Italy
Dr. Martí Gich, Science Institute of Barcelona (ICMAB), Spain
Dr. Jesus Garcia, Cales de Llierca, S.A., Girona, Spain
Prof. Andrés Ayuela, Materials Physics Center (CSIC-UPV/EHU) and DIPC associate, Spain

Invited Speakers
Prof. Aitor Bergara, Department of Condensed Matter Physics, University of the Basque Country (UPV/EHU) and DIPC associate, Leioa, Basque Country, Spain
Dr. Martijn Zwijnenburg, Materials and Inorganic Chemistry, University College London, London, UK
Dr. Scott Woodley, Materials Chemistry, University College London, London, UK
Dr. Javier Ruiz Fuertes, Departamento de Física Aplicada, Universitat de València, Valencia, Spain
Dr. Benjamin Morgan, Department of Chemistry, University of Bath, Bath, UK
Dr. Guillaume Ferlat, Institut de Minéralogie, Physique des Matériaux et Cosmochimie, Sorbonne Universités - UPMC Univ Paris 06, Paris, France
Dr. Stefano Leoni, Cardiff University, Cardiff, UK

Contributions
Dr. Javier Carrasco, CIC Energigune, Miñano, Basque Country, Spain
Dr. Thanayut Kaewmaraya, Institut d'Électronique Fondamentale, Université Paris-Sud, Orsay, France
Mr. Henry Hay, Institut de Minéralogie, Physique des Matériaux et Cosmochimie, Sorbonne Universités - UPMC Univ Paris 06, Paris, France
Mr. Daniel W. Davies, Centre for Sustainable Chemical Technologies and Department of Chemistry, University of Bath, Bath, UK
Dr. Rafael Grande-Aztatzi, Donostia International Physics Center (DIPC), Basque Country, Spain
Mr. Daniel W. Davies, Centre for Sustainable Chemical Technologies and Department of Chemistry, University of Bath, Bath, UK
Dr. Romain Dupuis, Donostia International Physics Center (DIPC), Donostia, Basque Country, Spain
Dr. Silvio Pipolo, IMPMC, Université Pierre et Marie Curie, Paris, France

Software Carpentry

June 27-29, 2016
Ignacio M. Barriola Center, CFM-UPV/EHU, Donostia / San Sebastián
http://cfm.ehu.eus/sc16

Organizing Committee
Iñigo Aldazabal Mensa (CFM (CSIC-UPV/EHU))
Andrés Diaz-Gil (Instituto de Física Teórica (CSIC-UAM), Madrid)
Diego Lasa (DIPC)

Helpers: Oier Echaniz, Ivor Loncaric, David de Sancho, Daniel Franco (DIPC), Brendan Costello, Ainhoa Bastarrika, Irene Monsalve, Iker Blanco

Software Carpentry's mission is to help scientists and engineers get more research done in less time and with less pain by teaching them basic lab skills for scientific computing. This hands-on workshop covered basic concepts and tools, including program design, version control, data management, and task automation. Participants were encouraged to help one another and to apply what they have learned to their own research problems.

On-Surface Synthesis International Workshop

June 27-30, 2016
Miramar Palace, Donostia / San Sebastián
http://oss.dipc.org/

Organizing Committee
Dimas G. de Oteyza (Ikerbasque, DIPC) (chair)
Celia Rogero (CFM (CSIC-UPV/EHU), DIPC)
Guillaume Vasseur (DIPC)
J. Enrique Ortega (UPV/EHU)
Daniel Sánchez-Portal (CFM (CSIC-UPV/EHU), DIPC)
José Ignacio Pascual (CIC nanoGUNE)
Karmela Alonso Arreche (DIPC)

Scientific Committee
André Gourdon (CEMES-CNRS, France)
Johannes Barth (Technische Universität München, Germany)
Trolle René Linderoth (Aarhus University, Denmark)
Nian Lin (The Hong Kong University of Science and Technology, Hong Kong)

On-surface synthesis unites the easy tunability of molecular materials and the promises of self-assembly as a revolutionary production method, with the sturdiness of covalently bonded structures. Because this approach bridges across the fields of chemistry, physics and materials science, the aim of this second edition of the "On-Surface Synthesis" international workshop was to bring together researchers working in this field from different perspectives.

Invited Speakers
Mike Crommie, University of California at Berkeley, USA
Roman Fasel, EMPA, Switzerland
Wei Xu, Tongji University, China
Florian Klappenberger, Technische Universität München, Germany
Guillaume Schull, IPCMS de Strasbourg (CNRS—Université de Strasbourg), France
Diego Peña, Universidad de Santiago de Compostela, Spain
Rasmita Raval, University of Liverpool, Great Britain
Dmitrii Perepichka, McGill University, Canada
Jonas Björk, Linköping University, Sweden
Daniele Passerone, EMPA, Switzerland
Steven de Feyter, KU Leuven, Belgium
Mauro Sambi, University of Padova, Italy

Interfacial Spintronics and Spin Waves

July 18-22, 2016
DIPC, Donostia / San Sebastián

Organizing Committee
Roberto Raimondi (University of Roma Tre)
Ilya Tokatly (UPV/EHU)
Sebastian Bergeret (CFM (CSIC-UPV/EHU), DIPC)
Giovanni Vignale (University of Missouri)

The workshop brought together theorists and experimentalists working on the fundamental physics of spin-charge conversion at interfaces between metals, insulators, magnets, and superconductors, the spin Hall effect and the anomalous Hall effect, anisotropic magneto-resistance, spin transfer torque, spin pumping, and spin wave control by electric, magnetic, and optical means. The workshop consisted of daily lectures followed by ample time for discussion.

Invited Speakers
Gerrit Bauer (Sendai)
Detlef Beckmann (Karlsruhe)
Felix Casanova (San Sebastian)
Miguel A. Cazalilla (Hsinchu)
Albert Fert (Paris)
Michael Flatte (Iowa)
Pietro Gambardella (Zürich)
Francesco Giazotto (Pisa)
Tero Heikkilä (Jyväskylä)
Timo Kuschel (Groningen)
Marta Luengo-Kovac (Michigan)
Florent Perez (Paris)
Jason Robinson (Cambridge)
Eiji Saitoh (Tohoku)
Ka Shen (Delft)
Eugene Sherman (Bilbao)
Jairo Sinova (Mainz)
Zhe Yuan (Beijing)
Shufeng Zhang (Arizona)
Shulei Zhang (Missouri)

Evaluation of Scientific Research and Iniciatives for Researcher's Support

July 19-20, 2016
Miramar Palace, Donostia / San Sebastián
https://www.uik.eus/es/evaluacion-de-la-actividad-investigadora-e-iniciativas-de-apoyo-al-investigador

Euskampus Foundation and DIPC organized this workshops with the aim of confronting and sharing experiences related to the quantitative evaluation of scientific activity. The two day workshop focused in the adequate use of bibliometric indicators and identification of the main institutions that develop evaluation processes at different levels and methodologies in our environment. The course methodology is based in Leiden´s Manifest.

The course was distributed into four sections:
Research Evaluation
Beyond the Impact Factor
Tupport Services to Research and Bibliometry Unities
¿How metrics affect scientific system?

Organizing Committee
Susana Sánchez-Gil (Euskampus) (chair)
Igor Campillo (Euskampus, DIPC)
Ricardo Diez (CFM CSIC-UPV/EHU, DIPC)

Opening
Iñaki Goirizelaia (Rector in the UPV/EHU, President of Euskampus Fundazioa)
Pedro Miguel Etxenike Landiribar (Professor in the UPV/EHU and President of DIPC)

Invited Speakers
Fernando Cossio, Ikerbasque
Julio Bravo de Pedro, ANEP
Eva Ferreira, UNIBASQ
Antonio Huerta, ICREA
Julieta Barrenechea, Euskampus Fundazioa
Miguel García, Thomson Reuters
Montserrat Hidalgo, Servei de Biblioteques, Public. i Arxius Universitat Politécnica de Catalunya
Isabel Iribarren, Maestro Biblioteca de la Universidad de Navarra
Marian Piñeiro, Biblioteca UPV/EHU
Juan Gorraiz, Library and archive services. Universität Wien
Fatima Pastor Ruiz, Sgiker. Universidad del País Vasco / Euskal Herriko Unibertsitatea
María José Rodriguez Tojo, Sgiker. UPV/EHU
Daniel Torres Salinas, EC3metrics Spin-off
Domingo Docampo, Universidade de Vigo
Elías Sanz Casado, LEMI-INAECU. Universidad Carlos III de Madrid
Evaristo Jiménez Contreras, Grupo EC3. Universidad de Granada
Rodrigo Costas Comesaña, CWTS. Universiteit Leiden

Spin-on Surfaces (SoS)

September 5-9, 2016
Miramar Palace, Donostia / San Sebastián

Organizing Committee
Deung-Jang Choi (CIC nanoGUNE)
Fernando Delgado (CFM (CSIC-UPV/EHU), DIPC)
Nicolás Lorente (CFM (CSIC-UPV/EHU), DIPC)

The Scanning Tunneling Microscope is giving unprecedented insight into magnetic phenomena on the atomic scale. The objective of this meeting was to share the state-of-the-art among the main actors in this field, as well as among interested students/researchers in related areas.

The covered material was:
• Single-atom magnetic inelastic spectroscopy.
• Single-molecule magnetic inelastic spectroscopy.
• Localized moments on different substrates: metals, insulators, superconductors, topological insulators.
• Spin dynamics on adsorbed atoms: T1 and T2 measurements and calculations.
• Electron spin resonance on a single atom.
• The Kondo effect.
• Entanglement in few-atom systems.
• Qubits on the atomic scale.

Invited Speakers
Jean-Pierre Gauyacq (Université Paris-Saclay & CNRS, France)
Samir Lounis (Jülich Research Centre, Germany)
Manuel Dos Santos Dias (Jülich Research Centre, Germany)
Joaquin Fernandez Rossier (INL, Portugal)
Katharina Franke (Freie Universität, Germany)
Jérémie Gobeil (TU Delft, Netherlands)
Harald Brune (EPFL, Switzerland)
Julen Ibanez (Jülich Research Centre, Germany)
Jens Wiebe (Universität Hamburg, Germany)
Floris Kalff (TU Delft, Netherlands)
Alexander Khajetoorians (Radbout University, Netherlands)
Jose Lado (INL, Portugal)
Laëtitia Farinacci (Freie Universität, Germany)
Benjamin Heinrich (Freie Universität, Germany)
Christian Ast (Max Planck Stuttgart, Germany)
Daniela Rolf (Freie Universität, Germany)
Sebastian Loth (Max Planck Hamburg, Germany)
Markus Ternes Max Planck (Stuttgart, Germany)
Martin Wenderoth Göttingen (Universität, Germany)
Maria del Carmen Marntinez Velarte (TU Delft, Netherlands)
Max Hänze (Universität Hamburg, Germany)
Gregory McMurtrie (Max Planck Hamburg, Germany)
Mohamad HicAhbadmo (Max Planck Hamburg, Germany)
Olof Peters (Freie Universität, Germany)
Sander Otte (TU Delft, Netherlands)
Pascal Ruffieux (EMPA, Switzerland)
Robert Sophus Drost (Max Planck Stuttgart, Germany)
Steffen Rolf-Pissarczyk (Max Planck Hamburg, Germany)
Carmen Rubio Verdù (nanoGUNE, Spain)
Shiyong Wang (EMPA, Switzerland)
Ranko Toskovic (TU Delft, Netherlands)

Topological States of Matter

September 5-9, 2016
Miramar Palace, Donostia / San Sebastián

Organizing Committee
Leonid Glazman (Yale University)
Felix von Oppen (Freie Universität Berlin)
Roman M. Lutchyn (Microsoft Station Q, University of California)
F. Sebastian Bergeret (CFM (CSIC-UPV/EHU), DIPC)
Vitaly N. Golovach (CFM (CSIC-UPV/EHU), DIPC)

The workshop focused on the topologically ordered phases of matter, their experimental signatures, and their possible applications for topologically-protected quantum computations. The goal of the workshop was to bring together leading experts, experimentalists and theorists, working on topological mesoscopic superconductivity. The workshop helped to foster collaborations in this new and rapidly developing field, important for the fundamental physics and applications.

Topological quantum matter represents a new class of materials which are characterized by non-local topological properties emerging from purely local (microscopic) degrees of freedom. Our understanding of topological states of matter has been broadened enormously over the last decade. The progress on the theoretical end includes, for example, the prediction of topological insulators and superconductors as well as the exploration of the interplay between symmetry and topology with an aim to classify topological states. A remarkable progress has been also made on the experimental front. Inspired by the theoretical predictions, experimentalists in laboratories across the world are now trying to realize the simplest topological quantum states. Among them much attention attracted Majorana systems, e.g. superconductors that support Majorana zero-energy modes (Majoranas). It is believed that the defects carrying these modes obey non-Abelian statistics and, as such, might be of potential use for quantum computing. There has been remarkable experimental progress in the quest to find Majoranas in various superconducting heterostructures involving semiconducting wires, ferromagnetic chains, and quantum spin Hall materials.

Invited Speakers
Ramón Aguado (ICMM/CSIC)
Alexander Altland (Univ of Cologne)
Carlo Beenakker (Leiden Univ)
Erez Berg (Weizmann)
Andrei Bernevig (Princeton Univ)
Parsa Bonderson (Station Q)
Piet Brouwer (Berlin Free Univ)
Evgueni Chulkov (DIPC, EHU)
Reinhold Egger (Duesseldorf Univ)
Silvano De Franceschi (CEA)
Sergey Frolov (Pittsburgh Univ)
Liang Fu (MIT)
Francesco Giazotto (CNR & SNS Pisa)
Manuel Houzet (CEA)
Jelena Klinovaja (Basel)
Leo Kouwenhoven (TU Delft)
Daniel Loss (Basel)
Charles Marcus (NBI)
Nadya Mason (UIUC)
Chetan Nayak (Station Q)
Yuval Oreg (Weizmann Inst)
Gil Refael (Caltech)
Jay Sau (Maryland Univ)
Ivo Souza (DIPC, CFM/EHU)
Ady Stern (Weizmann Inst)
Seigo Tarucha (Univ of Tokyo)
Björn Trauzettel (Wuerzburg Univ)
Jonas Wiedenmann (Wuerzburg Univ)
Amir Yacoby (Harvard Univ)
Ali Yazdani (Princeton Univ)

Contributions
Jennifer Cano (Princeton)
Gleb Finkelstein (Duke Univ)
Kam Tuen Law (Hong Kong)
Dganit Meidan (Ben-Gurion Univ)
Susanne Mueller (ETH Zürich)
Yuli Nazarov (TU Delft)
Fabrizio Nichele (Univ of Copenhagen)
Falko Pientka (Harvard University)
Patrik Recher (TU Braunschweig)
Michael Wimmer (TU Delft)

Physis Kai Polis. XII International Ontology Congress

October 3-7, 2016
San Sebastian
October 10-11, 2016
Barcelona

Organized by the Universität Autonoma de Barcelona, University of the Basque Country (UPV/EHU), Museo Chillida Leku and Paideia Galiza Fundación.

Scientific Committee
A. Aspect (Paris)
P. Aubenque (Paris)
F.J. Ayala (California)
J. Bouveresse (Paris)
E. Chillida (San Sebastián)
A. Grünbaum (Pittsburgh)
W. Lamb (Arizona)
T. Marco (Madrid)
U. Moulines (München)
I.Prigogine (Brussels)
H. Putnam (Boston)
C. Rovelli (Marseille)

In close collaboration with Donostia / San Sebastián European Capital of Culture 2016, the International Ontology Congress, whose biennial editions have been sponsored by UNESCO, focused its 2016 edition on reflecting on the relationship between Physis and Polis, a tribute to Aristotle in the 24th centenary of its birth and in the evocation of the dual project that summarizes Greek thought.

Pedro Miguel Echenique, president of DIPC, was the honorary president of this new edition of the International Ontology Congress which brought together eminent public figures from both the worlds of philosophy and of science.

The conference took place in two cities: in Donostia / San Sebastián from the 3rd through the 7th of October and in Barcelona on the 10th and 11th of October. The Faculty of Philosophy and Education (UPV/EHU) was the main venue in San Sebastián.

Invited Speakers
Christopher Fuchs (University of Massachusetts, Boston)
David Albert (Columbia University, New York)
David Wallace (University of Oxford, Balliol College)
François Englert (Nobel Prize of Physics 2013, Brussels)
Harvey Brown (University of Oxford, Fellow of the British Academy)
Alberto Bernabé (Chair of Greek Philology, Madrid)
Carlo Natali (Università Ca' Foscari, Venice)
Demetra Sfendoni-Mentzu (President of the Interdisciplinary Centre for Aristotle Studies, Thessaloniki)
Gabriele Cornelli (Universidade de Brasília, President of the International Plato Society)
Tomás Calvo (International Federation of Philosophical Societies, Madrid)
Anna Estany (Barcelona, Universitat Autònoma de Barcelona)
Dermont Moran (President of the FISP, Edward Goodwin Ballard Prize in Phenomenology, Dublin)
Francisco J. Ayala (Templeton Prize, Irvine)
Ulises Moulines (Ludwig-Maximilians-Universität, Munich)
Fernando Savater (San Sebastián)
Ioanna Kuçuradi (UNESCO Chair of Philosophy of Human Rights, Istambul)
Luca Scarantino (IULM Milano)
Supakwadee Amatayakul (Chulalongkorn University)
Victoria Camps (Autonomous University of Barcelona)

Workshop on Strong Coupling with Organic Molecules

October 19-21, 2016
Miramar Palace, Donostia / San Sebastián
http://scom16.dipc.org/

Organizing Committee
Bill Barnes (University of Exeter, UK)
Francisco García Vidal (Universidad Autónoma de Madrid and DIPC, Spain)
Jaime Gómez Rivas (Eindhoven University of Technology and
Dutch Institute for Fundamental Energy Research, Netherlands)
Javier Aizpurua (Center for Materials Physics, CSIC-UPV/EHU and DIPC, Spain)

This workshop brought together researchers from different disciplines including: Photonics, Quantum Optics, Materials, Chemistry and Condensed Matter Physics to discuss the latest developments in the study of the strong coupling involving organic molecules and optical cavities. Leaders in the field discussed recent results on phenomena that involve polaritonic states, molecular excitations, molecular vibrations and their complex interactions, giving raise to a plethora of fascinating effects of both scientific and technological interest. Our aim was that this meeting should act as a catalyst in this emerging field, encouraging discussion of the underlying concepts and promoting new directions and collaborations.

Invited Speakers
Harry Atwater (Caltech, USA)
Jeremy J. Baumberg (Cambridge, UK)
Joel Bellesa (Lyon, France)
Jacqueline Bloch (CNRS, France)
Thomas Ebbesen (Strasbourg, France)
Bert Hecht (Wurzburg, Germany)
Jonathan Keeling (St. Andrews, UK)
David Lidzey (Sheffield, UK)
Christoph Lienau (Oldenberg, Germany)
Brahim Lounis (Bordeaux, France)
Martin Plenio (Ulm, Germany)
Said Rodriguez (CNRS-LPN, France)
Salvatore Savsta (Messina, Italy)
Timur Shegai (Chalmers, Sweden)
Blake Simpkins (NRL, USA)
Frank Spano (Temple university, USA)
Paivi Torma (Aalto, Finland)

Transborder Theoretical Chemistry Days

November 9-10, 2016
Bayonne, France

Organizing Committee
Pascal Larregaray (Université de Bordeaux)
Xabier López (UPV/EHU, DIPC)

Theoretical Chemistry and Physics at the Quantum Scale (QuantumChemPhys) is a Transborder Joint Laboratory (LTC - Laboratoire Transfrontelier Conjoint) created by Université de Bordeaux (UBx), Universidad del País Vasco / Euskal Herriko Unibertsitatea (UPV/EHU), and Donostia International Physics Center (DIPC). The purpose of the QuantumChemPhys lab is to strengthen the scientific collaboration among researchers from Euskadi and Aquitaine through the creation of a transnational institution focusing on the theoretical aspects of chemistry and physics at the quantum scale, i.e. the quantitative description of the motion of electrons and nuclei (and their coupling) in solids, at gas-solid interfaces, as well as in the interaction with light. Such a challenge requires the developments of theoretical methods and numerical simulations within the framework of quantum/classical/semiclassical mechanics.

In this context, on November 9th and 10th, the QuantumChemPhys lab organized the Transborder Theoretical Chemistry Days, in which researchers mostly working in theoretical chemistry joined to share their expertise in the field and explore the possibilities of further collaboration. Approximately 30 scientists from the three institutions forming the QuantumChemPhys lab gathered in Bayonne.

Contributions
Daniel Sanchez Portal
Lionel Truflandier
Eduard Matito
Alain Fritsch
Mario Piris
Ion Mitxelena
David Casanova
Frédéric Castet
Claire Tonnelé
Jon M. Matxain
Jon Uranga
Angelos Giannakopoulos
Nicolas Lorente
Fabio Busnengo
Andres Arnau
Laure Lespade
Xabier Lopez
Rafael Grande-Aztatzi
Katarzyna Brymora
Micaela Matta
Sai Manoj Gali
Oihana Galparsoro
Alejandro Pena Torres
Cedric Crespos

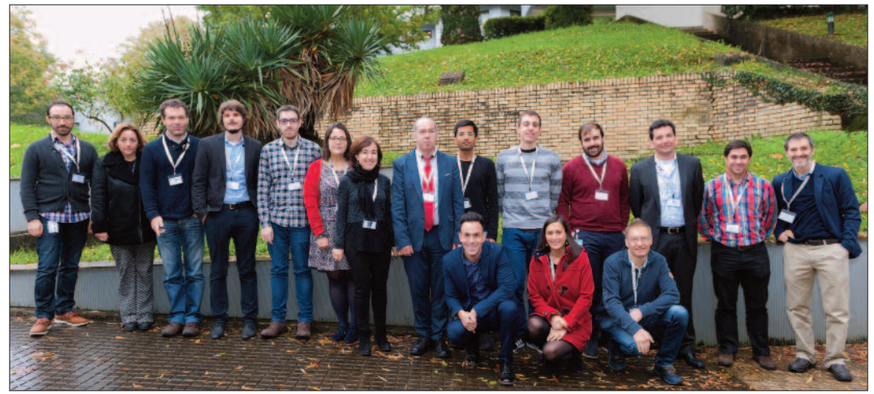
5th BASKRETE Open Days to Industry

November 10-11, 2016
DIPC, Donostia / San Sebastián

Organizing Committee
Jorge S. Dolado (Tecnalia)
Romain Dupuis (DIPC)
Silvina Cerveny (CFM CSIC-UPV/EHU)
Hegoi Manzano (UPV/EHU)
Andres Ayuela (CFM CSIC-UPV/EHU, DIPC)

The BASKRETE initiative is a collaborative project within the Campus of International Excellence Euskampus carried out between the University of the Basque University (UPV/EHU), the Materials Physics Center (CFM), the Donostia International Physics Center (DIPC) and TECNALIA with a twofold mission: on one hand, BASKRETE coordinates all the actions which are currently underway in the Basque Country in the field of nanoscience and nanotechnology for cementitious materials and, on the other hand, BASKRETE aims to trigger the transfer of high technology knowledge to companies through the establishment of a cooperative program with the industrial agents.

Contributions
A. Martinez Muro (SPRI)
J.S. Dolado (TECNALIA R&I)
M. Diez (UPV/EHU & University Bordeaux)
A. Santamaria (UPV/EHU)
R. Dupuis (DIPC)
H. Manzano (UPV/EHU)
A. Ayuela (DIPC)
A. Prabhu (TECNALIA R&I)
G. Goracci (MPC)
P. Martin (TEC R&I)
A. Bonnet (SUMICOL)
J. Gomez (ADVANCED MATERIAL SIMULATION SL)
O. Kutluoglu (QWIKSEED LT)
A. Balza (Intevep-PDVSA)
S. Martinez (IEM-CSIC)
E. Goiti (TECNALIA R&I)
I. Vegas (TECNALIA R&I)
I. Emaldi (POLYMAT)
E. Duque (UPV/EHU)
A. Orbe (UPV/EHU)
V. Garcia (TECNALIA R&I)



Higher Education

DIPC School

Nanotechnology meets Quantum Information - NanoQI

July 11-14, 2016
Miramar Palace, Donostia / San Sebastián
http://nanoqi.dipc.org/

Organizing Committee
J. Ignacio Cirac (MPQ Garching, Germany)
Geza Giedke (Ikerbasque, DIPC)
Alejandro González-Tudela
Ataç Imamoglu
Mikhail Lukin

Ever smaller and better designed structures for sensing and computing are reaching the quantum realm, leading to new promises and challenges in information processing. The school "Nanotechnology meets Quantum Information" aimed to provide a broad overview of different implementations of quantum information processing and quantum simulation enabled by recent progress in nanotechnologies.

Seven leading experts reviewed the experimental and theoretical state-of-the-art for some of the most promising implementations such as semiconductor quantum dots, superconducting circuits, defect centers in diamond, photonic crystal structures, and topological insulators and explored the prospects of quantum computing, quantum simulation, and the physics of quantum many-body systems.

Invited Speakers
Darrick E. Chang (ICFO Barcelona, Spain)
J. Ignacio Cirac (MPQ Garching, Germany)
Liang Fu (MIT Cambridge, USA)
Atac Imamoglu (ETH Zurich, Switzerland)
Daniel Loss (University of Basel, Switzerland)
Mikhail D. Lukin (Harvard University, Cambridge, USA)
Andreas Wallraff (ETH Zurich, Switzerland)

DIPC School

Topological Matter School 2016

August 22-26, 2016
Miramar Palace, Donostia / San Sebastián
https://tms16.sciencesconf.org/

Organizing Committee
Dario Bercioux (Ikerbasque, DIPC)
M. Reyes Calvo (CIC nanoGUNE)
Maia G. Vergniory (DIPC)
François Konshelle (CFM (CSIC-UPV/EHU))

Topological states of matter consist in new platforms where quantum mechanics realizes at a mesoscopic scale. This emerging topic grew up impressively in the last few years: a few problems have been resolved (as the classification of non-interacting systems) whereas many more are still open questions.

The aim of this one week school was to introduce students to the recently developed field of topological states of matter. The main goal was to cover basic and advanced aspects of the field, including a set of lectures explaining practically how to perform a first principle approach to the problem.

Invited Speakers
Alexander Altland (University of Cologne)
Mois Aroyo (UPV/EHU Bilbao)
Andrei Bernevig (Princeton University)
Claudia Felser (Max Planck Dresden)
Titus Neupert (University Zürich)
Alexey Soluyanov (ETH Zürich)
Ivo Souza (CFM,UPV/EHU Donostia / San Sebastián)
Binghai Yan (Max Planck Dresden)

DIPC School

Dynapeutics

September 25-30, 2016
Miramar Palace, Donostia / San Sebastián
http://dynapeutics.dipc.org/speakers

Scientific Committee
Emanuele Paci (University of Leeds, UK)
Annick Dejaegere (Institut de Génétique et de Biologie Moléculaire et Cellulaire, Strasbourg, France)
Roland H. Stote (Institut de Génétique et de Biologie Moléculaire et Cellulaire, Strasbourg, France)
Michael Schaefer (Novartis Pharma AG)
Olivier Michelin (Université de Lausanne, Switzerland)
Vincent Zoete (Université de Lausanne, Switzerland)
Nathalie Reuter (University of Bergen, Norway)
Lennart Nilson (Karolinska Institutet, Stockholm, Sweden)
Thomas Simonson (Ecole Polytechnique, Paris, France)
Stefan Boresch (University of Vienna, Austria)
Darrin M. York (Rutgers University, New Jersey, USA)

Organizing Committee
Prof. Xabier Lopez (UPV/EHU, DIPC)
Dr. Jon I. Mujika (UPV/EHU, DIPC)
Dr. Elixabete Rezabal (UPV/EHU, DIPC)
Dr. Eider San Sebastian (UPV/EHU)
Dr. Elena Formoso (UPV/EHU, DIPC)
Dr. Rafael Grande-Aztatzi
Dr. Jose M. Mercero

DYNAPEUTICS international summer school aimed to introduce, describe and discuss the theory and applications of computational methods for the study of biological molecules, relevant for the understanding of design and optimization of molecular drugs, and for the understanding of biological processes in general at the molecular level. The school was taught at the postgraduate level and was addressed to PhD students and postdoctoral researchers with a solid background in biophysics.

The course consisted of several seminars and computation training that covered the main concepts introduced in the seminars. The school was part of a wider initiative "Passion For Knowledge" that attracted leading scientists from around the world to San Sebastian to share their research experience, like Nobel Laureate Prof. Martin Karplus. Hence, the participants also benefited from an outstanding atmosphere and social activities around the school that emphasized the links between science and society, in its most general sense.

Subjects covered in the school:
- Force fields
- Simulation methods overview
- Molecular Dynamics and Monte Carlo Methods
- Normal Mode Analysis
- Accelerated dynamics
- Free energy Calculations
- Continuum electrostatics
- Homology modeling
- Docking
- Drug design
- Quantum Chemistry and QM/MM methods

Invited Speakers
Martin Karplus (Harvard University and Université de Strasbourg)
Emanuele Paci (University of Leeds, UK)
Annick Dejaegere (Univ. of Strasbourg, France)
Roland H. Stote (Univ. of Strasbourg, France)
Michael Schaefer (Novartis Pharma AG, Switzerland)
Olivier Michielin (Swiss Institute of Bioinformatics, Switzerland)
Vincent Zoete (Swiss Institute of Bioinformatics, Switzerland)
Antoine Daina (Swiss Institute of Bioinformatics, Switzerland)
Nathalie Reuter (Univ. of Bergen, Norway)
Lennart Nilson (Karolinska Institutet, Stockholm, Sweden)
Leif A. Eriksson (Göteborgs Universitet, Göteborg, Sweden)
Ronen Zangi (Univ. of the Basque Country, Spain)
Stefan Boresch (Univ. of Vienna, Austria)
Darrin M. York (Rutgers University, New Jersey, USA)
Markus Meuwly (Univ. of Basel, Switzerland)
Jon I. Mujika (Univ. of the Basque Country, Spain)
Ferran Feixas (Univ. de Girona, Girona, Spain)
Pedro A. Fernandes (Univ. of Porto, Porto, Portugal)

Theses

Size-dependent electronic properties of metal nanoparticles.
Marina Quijada Van der Berghe
January 2016
Supervisors: Ricardo Díez Muiño and Pedro Miguel Echenique

Classical and quantum approaches to the interaction of light and matter at the nanoscale.
Mikolaj Kajetan Schmidt
January 2016
Supervisor: Javier Aizpurua

Electron dynamics in the interaction of atomic particles with spherical metal clusters.
Natalia Koval
April de 2016
Supervisor: Daniel Sanchez Portal

Phonon and electron excitations in abstraction processes from metallic surfaces.
Oihana Galparsoro Larraz
December 2016
Supervisors: Maite Alducin (UPV/EHU) and Pascal Larregaray (Université de Bordeaux)

Elementary reactive processes of nitrogen and hydrogen on metal surfaces: a theoretical study.
Mohamed Ahmed Mohamed Abdelazim Nosir
December 2016
Supervisor: Ricardo Díez Muiño

Master's Degree Program

UPV/EHU Research Master's in Nanoscience

DIPC collaborates in the official postgraduate program in nanoscience organized by the Materials Physics Department of the University of the Basque Country (UPV/EHU) and the Center of Materials Physics (CSIC-UPV/EHU) "Master's in Nanoscience".

The Research Master's in Nanoscience has been offered since 2007. More than eighty students have obtained their Master's degree. Almost 50% of our graduates are international students from four continents (Europe, America, Africa and Asia).

Researchers at DIPC participate in this program in various ways and from different perspectives by developing curriculums, giving lectures, acting as counselors to some of the students, and providing seminars on issues of special interest to the students.

In addition, DIPC plays a valuable role, providing essential infrastructure and funding, within its means, to help ensure the proper development of the program.

Credits

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