DIPC 2017

Donostia International Physics Center

ON THE COVER DANCING ELECTRONS LOSE THE RACE

Electrons photoemitted from subsurface layers of WSe_2 are strongly affected by intra-atomic interactions. After absorption of a photon, the electrons are dynamically confined by a centrifugal barrier and remain trapped for times in the attosecond scale. The motion of these electrons around the nuclei, before being eventually emitted, is kind of a dance. A combination of experimental and theoretical work shows that electrons that remain 'dancing' around the atom need longer times to reach the surface. The cover image shows an artist's rendition of this process.

Photography **López de Zubiria** | Art direction **Santos Bregaña** | Dancer **Itsaso Gabellanes**

Angular momentum-induced delays in solid-state photoemission enhanced by intra-atomic interactions
Siek F, Neb S, Bartz P, Hensen M, Struber C, Fiechter S, Torrent-Sucarrat M, Silkin VM, Krasovskii EE, Kabachnik NM, Fritzsche S, Diez Muino R, Echenique PM, Kazansky AK, Muller N, Pfeiffer W, and Heinzmann U. Science 357, 1274 (2017).

2017

DIPC ACTIVITY REPORT

DIPC: Coming of Age

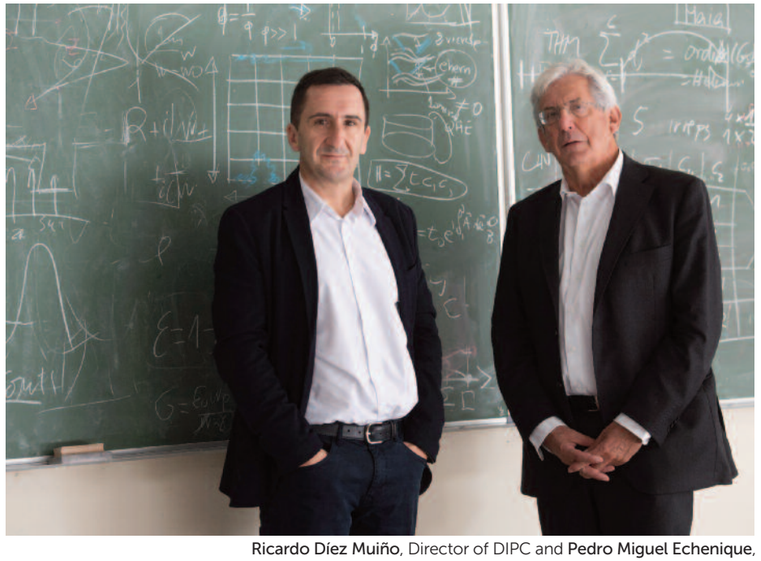
Donostia International Physics Center (DIPC) was effectively born on April 27th, 2000. On this date, **Heinrich Rohrer**, Nobel Laureate in Physics, delivered the opening lecture that set the commencement of activity in the center. Rohrer claimed in his talk that "the purpose of an international center is to bring science together from different cultures, of different thinking, and that is one of the very promising ways of approaching solutions to the complex issues of the future".

Like any other young creature, DIPC started its scientific life full of energy and enthusiasm. DIPC was eager to use science to disentangle the complexities of the world. In accordance with Rohrer's wisdom, DIPC became soon an international hub between the local community of researchers and a world-wide network of elite scientists. A constant flow of new ideas was obtained through a program of top-level visiting researchers who enjoyed complete freedom to go about their work. This dynamic atmosphere proved to make a direct impact in the quality of DIPC research as well as in its visibility and recognition.

Eighteen years later, DIPC has reached what is often considered the age of majority, the maturity as organism. *Coming of age* implies assuming further responsibility, careful thinking, and new projects. All this without losing the spirit that drives DIPC's personality. In the case of DIPC, planning for the future was also prompted by the external evaluation arranged every four years by the Department of Education of the Basque Government within the Basque Excellence Research Centers (BERC) Program. The BERC evaluation report, elaborated by an international scientific committee, highly praised the recent activity of DIPC, firmly endorsed the strategy for the period 2018-2021, and strongly encouraged to continue with the development of DIPC.

With age, changes arise

A relevant novelty in the life of DIPC will be diversification of the scientific activity. Until now, research lines at DIPC were mostly focused on several aspects of condensed matter physics and materials sciences, including the study of advanced materials, attophysics, surfaces and interfaces, photonics, plasmonics, quantum information, polymers, soft matter, biofunctional nanosystems,



Ricardo Díez Muiño, Director of DIPC and **Pedro Miguel Echenique**, President of DIPC since 2000.

and computational chemistry, among other topics. The singular structure of the DIPC research community, in which international visitors naturally collaborate with DIPC Researchers and Associates, is an extremely successful model to generate scientific knowledge of the highest level. The model can be fruitfully extended to other subdisciplines of physics. Hence, DIPC is launching new research lines on topics that were not previously included in the activity of the Center. Experimental particle physics and cosmology are the first research lines that will be added following this strategy.

This qualitative growth will be triggered by scientists of proven excellence, hired thanks to the invaluable support of Ikerbasque, the Basque Foundation for Science of the Basque Government. We are sure that the expansion to other fields of physics will enrich the research atmosphere of DIPC and stimulate the creativity of all scientists working here.

The growth of a creature naturally means the growth of some of its organs too. DIPC hosts an infrastructure that provides services to a large community of researchers, namely, the DIPC Supercomputing Center. Computational physics and chemistry is one of the strongest research lines in the Basque Country and the Supercomputing Center plays a key role in its development. Furthermore, the Center is instrumental to attract researchers to Basque research centers. The DIPC Supercomputing Center is currently expanding not only in size and power but also in scope: scientists affiliated to local research institutions other than DIPC are having access to the computational resources provided by this facility, which is additionally generating and keeping specialized expertise on high-performance computing.

Last but not least, DIPC will reinforce outreach activities. Science cannot and should never be regarded or interpreted without considering its human character. The development of science is intrinsically entangled with the evolution of society. At DIPC we are fully engaged in spreading the beauty of science and the usefulness of scientific knowledge, as well as sharing the joys and challenges of a life in science. So even after 18 years of life, DIPC researchers keep their curiosity and excitement about science. For us, especially when it comes to enthusiasm, there is no childhood's end. ■

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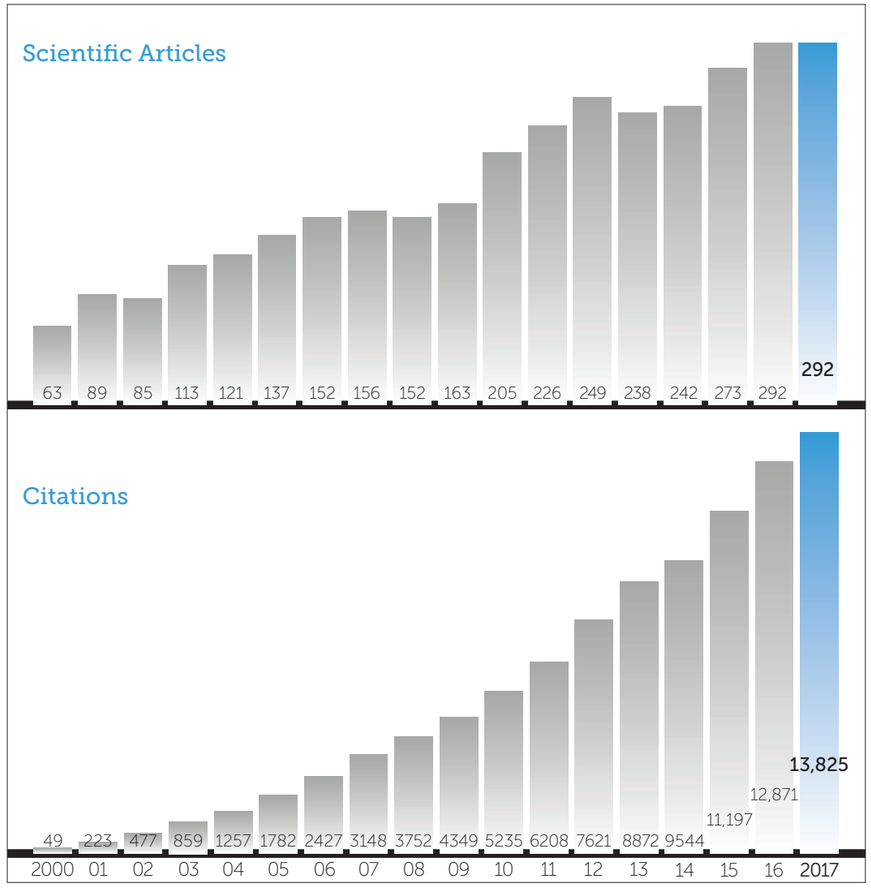
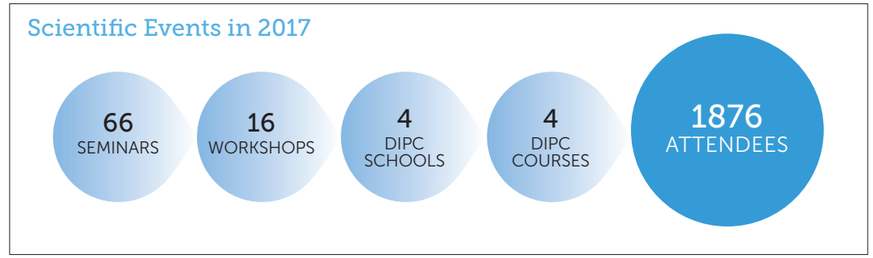
Research Activity at a Glance

DIPC's scientific production and international impact continues to increase. During the last 18 years, the center has published a total of **3,344 ISI publications** and has received more than **94,312 citations**. In 2017, **292 scientific articles** and **one book chapter** mean an **increase of 42%** in the number of publications since 2010.



Source Web of Science Core Collection (all years and indexes) - DIPC's Researcher ID C-3171-2014 (17/05/2018)



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 and Courses which focus on learning particular skills.

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

The core of the DIPC Community is made up of local scientists as well as PhD students and postdoctoral researchers who come from other institutions to complete their training and hone their expertise with us. DIPC Associates are situated in other centers at different faculties of the University of the Basque Country and at the Materials Physics Center. Our scientists act as hosts for the large number of international visiting researchers and retain the scientific-technical knowledge locally which helps to develop long term DIPC research projects. Among the local host community, there are also Ikerbasque Researchers and Gipuzkoa Fellows.

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.

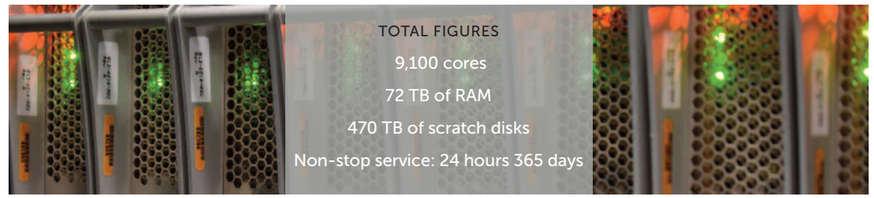
"The variety and power of the computing resources of DIPC, and its constant upgrade, allow the permanent confrontation of a wide range of numerical simulations that put DIPC at the forefront in research."

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 2017, the Center has 6 different supercomputers covering a wide range of computational needs, from Xeon E5-2680 V3 nodes with 24 cores, 128 GB of RAM and Infiniband FDR connection, large Xeon Platinum 8164 shared memory computers with 52 cores and 1.5 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 168 researchers from DIPC and other research centers such as the UPV/EHU, the CSIC-UPV/EHU Materials Physics Center, CIC nanoGUNE, BioDonostia and Ikerbasque used this computational infrastructure in 2017.

Science Communication

DIPC is fully committed to the dissemination and transfer of scientific knowledge to society because we believe that a more informed society is more prepared to take the decisions that will shape our future. To do so, we establish a fluid and permanent dialogue with society through our extensive outreach program.

Participants join the speakers in the foyer of Eureka! Zientzia Museoa at the 9th edition of top@DIPC Encounters

top@DIPC Encounters. Zientziarekin solasean!

DIPC organized the 9th edition of the annual Encounters between Nobel Laureates and leading researchers with high school students. 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.

30/10/2017
Eureka! Zientzia Museoa, Donostia

Albert Fert
Unité Mixte de Physique CNRS/Thales
Nobel Laureate in Physics 2007

Pilar Hernández
CERN, Theoretical Division

Angela Nieto
Instituto de Neurociencias de Alicante
Jaime I Prize in Basic Research (2009)

Presenter:
Nora Gonzalez (DIPC)
Moderator:
Pedro Miguel Etxenike (DIPC)

More than **325 students and teachers** from schools of Gipuzkoa, Bizkaia and Araba participated at this year's Encounter. As usual, **Telefónica**, a long-time patron of DIPC, collaborated by giving an award to the most innovative, creative, original, surprising or interesting question.

Seminars by Distinguished Scholars

High profile scientists and scholars are invited to DIPC to give a seminar and share their experience in science with young researchers and the general public in an informal manner.

05/05/2017
Chris Rossel
IBM Research & European Physical Society
From nanoscale systems to neuromorphic computing: a quick overview of S&T at IBM Research-Zurich

14/11/2017
Helmut Schwarz
Alexander von Humboldt Foundation (Germany)
The Methane Challenge - C–H Bond Activation by Metal Oxides: Theory and Experiment in Concert

Kutxa Lectures

The Kutxa Lectures, organized in collaboration with **Kutxa Fundazioa** in Donostia / San Sebastián, started in 2010. Speakers include Nobel laureates and other renowned scientists as well as science communicators and humanists working in the frontiers of science.

14/11/2017
Helmut Schwarz
Alexander von Humboldt Foundation, Germany
Useless Knowledge: Why is Funding of Basic Research Vital for Society?
Koldo Mitxelena, Donostia / San Sebastián

"New Ways of Science" Lectures

A cycle of talks organized jointly by **Ernest Lluch Cultural Center** from Donostia Kultura and DIPC in an attempt to bring our work closer to society. Scientists from DIPC introduce the fundamentals of Materials Science and historical milestones in a clear and attractive way to the general public.

26/10/2017
Celia Rogero
Researcher at the Materials Physics Center (CFM CSIC-UPV/EHU)
Ciencia de superficie:
la vida secreta de las moléculas

Special Lecture in Ondarroa

In collaboration with **Zientziaren Giltzak Association**, in 2017 we organized a very special lecture in Ondarroa to support the great science dissemination activity that the association is carrying out in the small coastline village. The event was presented by Pedro Miguel Echenique.

31/10/2017
Pilar Hernández Gamazo
Theoretical Physicist at CERN
CERN: Una ventana al universo

High School Visits

In 2017, DIPC together with the Materials 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 up close.

During 2017 DIPC and CFM hosted a total of 540 students from 13 schools.

13/01/2017	San Benito Ikastola	28/04/2017	Koldo Mitxelena BHI
27/01/2017	Zubiri Manteo Institutua	06/10/2017	La Anunciata Ikastetxea
10/02/2017	Summa Aldapeta	03/11/2017	Urola Garaiko Lanbide Eskola
23/02/2017	Usandizaga Institutua	17/11/2017	IES Arrasate BHI
10/03/2017	Toki Ona BHI	23/11/2017	UROLA ERASMUS
24/03/2017	Colegio de la Asunción	15/12/2017	IES Bidebieta BHI Donostia
07/04/2017	Laskorain Ikastola		

On Zientzia

14/06/2017
The award ceremony of the seventh edition of the On Zientzia video contest organized jointly by DIPC and **Elhuyar Foundation** took place at the headquarters of Kutxa Kultur Plaza at Tabakalera. The event was later broadcast on *Teknopolis,* a local TV program. In this year's edition, 87 videos were entered into the contest.

The awardees were:

BEST DISSEMINATION VIDEO
Keats vs Feynman
Patxi Razkin Senar (Engineer at CAF)

BEST VIDEO IN BASQUE
Arrazak
Alfonso Larrazabal and **Unai Unda**
(Audiovisual professionals)

YOUNG PRIZE
Fallos científicos en el cine
Mario Martínez Saénz (15 years old)

SPECIAL MENTIONS
Piztu Argia
Faraday Gazteak (5-8 years old)
El frustrante viaje de un átomo de carbono
Julio Ruiz Monteagudo (secondary school teacher in Slovakia)

For more information visit:
www.onzientzia.tv

DIPC Science Dissemination Contest

Organized annually since 2015 in collaboration with the well-known Spanish cultural magazine *Jot Down*, the dissemination contest recognizes the best science dissemination articles.

The prize-giving ceremony of this third edition took place at the annual encounter that Jot Down Science celebrated in Sevilla on the 23th of September.

FIRST PRIZE
Un golem movido por bacterias
Martín Sacristán

FINALISTS
2nd: *Borre sólo este recuerdo, por favor*
María del Carmen Martín-Buro
3rd: *El nacimiento de una metáfora*
Iván Rivera
4th: *Insectos Zombis*
Pablo José Barrecheguren Manero
5th: *Pinto así porque puedo*
Deborah García Bello

LANALDI

26/05/2017
Organized every year by **Novia Salcedo Foundation**, DIPC researchers and professionals participate by hosting a student for a day, and showing the student what the work of a scientist or a communicator is like.

Physicist: **Arantza Garcia Lekue**
Participant student: **Uxia Intxausti**

VIDAS CIENTÍFICAS

23/10/2017
Eureka! Zientzia Museoa organizes every year a full-day event for young students where some of our researchers participate with a talk or a poster about their work or research.

Nuevos nanomateriales para uso en fotoquimioterapia
Juan Gurruchaga Pereda

Síntesis y caracterización de poliéteres cíclicos regioregulares
Jordan Ochs

Science Week

Stand in Tabakalera
09-11/11/2017
Tabakalera, Donostia / San Sebastián

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 Material's World* at Science Week organized by the **University of the Basque Country (UPV/EHU)**. In addition to the stand, there was an exhibit: *Dayanne and Murillo. The power of nanoscience*.

Zientzia Club
Some of our researchers and communicators participated in Zientzia Club organized within the Science Week events. They gave amusing scientific monologues in the Basque Country celebrated on two occasions:

November 9th in Centro Cívico Clara Campoamor, Barakaldo
November 11th in Tabakalera, Donostia / San Sebastián

Arraultz fluoreszenteak
Txoni Matxain

Landare nanohibridoak
Amaia Arregi

nanoKOMIK

After the success reaped in 2016, the second edition of the nanoKOMIK challenge organized by DIPC and CIC nanoGUNE was launched at the beginning of 2017. This second edition involved more than 240 participants over 14 years of age who took part in a free creative process 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). In 2017, **Itxasne Azpitarte** and **Jose Carlos Torre** participated along with several researchers of our centers in the project.

nanoKOMIK challenge
The second edition of nanoKOMIK has introduced a new age category allowing adults to participate on the challenge, and giving the winners the possibility to participate in the creation of the collective nanofiction work. The 57 artworks presented are visible on our website.

Science and Comic Workshops
Science and comic workshops guided by cartoonists, scientists and science communicators were organized again in schools, museums and public libraries to encourage people to participate in the challenge. A special seminar to encourage young artists to participate in the adult age category was in addition organized in the Faculty of Fine Arts of the University of the Basque Country (UPV/EHU). The list of the organized workshops follows:

04/04/2017	Special Seminar for teachers at DIPC (Donostia / San Sebastián)
02/05/2017	IES Mungia, Mungia (Vizcaya)
02/09/2017	Colegio Irlandesas, Lejona (Vizcaya)
25/04/2017	CosmoCaixa (Barcelona)
11/04/2017	Faculty of Fine Arts of the University of the Basque Country (UPV/EHU)
25/04/2017	Ignasi Iglésias-Can Fabra Public Library (Barcelona)

Itinerant exhibition

In 2017, the exhibition of the 2016's collective comic *Dayanne and Murillo. The power of Nanoscience* travelled throughout the Basque Country and Cataluña.

Award 2017
The awards were submitted by the formal jury and made public in the project's website and social networks:

FIRST PRIZE
QUBLINGS - the espionage mission to Pluto
Aśka (Perth, Australia)

SECOND PRIZE
Teknaria
Jose Sénder-Quintana (Barcelona)

The winning comics were published in Jot Down's journals sold along with the well-known *El Pais* newspaper.

Category for teenagers:
FIRST PRIZE
Besaluze
Jonas Casado-Etxeberria (Hernani)

SECOND PRIZE
Kasu inurriekin
Maricielo Asto-Huaman (Bera)

People's choice award:
Hackgirl
Rubén Molina (Barcelona)

Publication of the Collective Nanofiction Comic

Using the best ideas from the comics submitted for the challenge as a point of reference, and in collaboration with the winners of the general category, three new nanocomics were produced.

The comic was presented in Komikigunea on January 23rd together with the itinerant exhibition of both editions and distributed to all participants as well as the public libraries in the Basque Country. It is also available in Basque, Spanish, French and English on the nanoKOMIK website.

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

Mestizajes

Besides traditional forms of knowledge, DIPC also explores alternative spaces lying at the boundaries among different disciplines. *Mestizajes* is a transdisciplinary program coordinated by **Gustavo Ariel Schwartz** that bridges the gap between artistic, social and scientific branches of 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

28/03/2017
Centro Cultural Ernest Lluch
Donostia / San Sebastián
Conectando mundos las redes complejas dentro y fuera de la ciencia
Ricard Solé
Universidad Pompeu Fabra, Barcelona

21/07/2017
DIPC, Donostia / San Sebastián
Science and Contemporary Theater: A symbiotic relationship?
Gabriel Cwilich
Yeshiva University, New York

International Conference on Literature and Science

23- 25/10/2017
Donostia / San Sebastián

III International Conference on Literature and Science: Matter, Life and Consciousness from Science and Literature was organized within the framework of the Mestizajes program, presenting a number of invited talks opened to both professionals and the general public. The aim of the Conference was to pursue a journey of 13.8 billion years of cosmic evolution that has turned matter into life and consciousness. With this in mind, *Mestizajes* proposed an interdisciplinary perspective that crossed the limits of knowledge between literature and science. During the meeting, there were two types of activities programmed: a workshop aimed at people in the academic field in the mornings at DIPC headquarters; and a cycle of open public lectures in the afternoon at San Telmo Museum.

Publication of the book #Nodos

23- 25/10/2017
Donostia / San Sebastián

#Nodos is an intellectual adventure that explores the boundaries among different areas of knowledge. #Nodos is a transdisciplinary meeting point where artists, scientists, writers and humanists from different countries share experiences and reflections on the relevance and possibilities of the interaction among different disciplines. It is a book that brings together about 100 contributions from people from different countries from the field of science, humanities, literature and art around ten thematic areas: *Complex Networks, Metaphor, Cosmos, Chaos and Complexity, Emergency, Perception, Memory, Emotion, Consciousness and Big data*. The edition of the book has been coordinated by **Gustavo Ariel Schwartz**, tenured scientist from CFM and associated to DIPC, and **Víctor Bermúdez** and is an excellent example of a transdisciplinary research space. The book has been published by Next Door Publishers and is available in bookstores and on-line. The first edition of the book was sold out in three months. The English version of the book is expected to be published some time in 2018.

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

In Praise of Science and Culture

Pedro Miguel Echenique, president of DIPC, has played an active role in raising awareness of the necessity and importance of basic research for the development of society. In 2017 Professor Echenique delivered 17 lectures locally and internationally.

02/02/2017 **La sublime utilidad de la ciencia inútil** Santiago de Compostela

02/14/2017 **Ciencia. Economía. Cultura. La riqueza de las nociones**
Encuentros CIVICAN, Pamplona

02/23/2017 **Ciencia. Educación. Futuro.** Colegio Summa Aldapeta, Donostia / San Sebastián

03/04/2017 **History of the 3S** Symposium on Surface Science 2017 (3S'17), St. Moritz, Switzerland

04/18/2017 **La sublime utilidad de la ciencia inútil** VI Congress ScienceIES, Sevilla

05/02/2017 **Diálogos sin fronteras** Médicos sin frontera, CIVICAN, Pamplona

06/26/2017 **Ciencia. Cultura. Progreso.**
"Divulgación y cultura científica: diálogo universidad/sociedad", UIMP, Santander

07/06/2017 **The sublime utility of useless Science**
"Structure and Dynamics of Internal Interfaces" Colloquium, Philipps-Universität Marburg

09/15/2017 **La sublime utilidad de la ciencia inútil** XXVI Encuentros Humboldt, Málaga

09/23/2017 **Ciencia. Cultura. Economía. Belleza.**
Colegio Mayor Ayete, Donostia / San Sebastián

10/06/2017 **Ciencia y belleza** Tribute to Prof. Martí Massó, Hospital Donostia

10/10/2017 **Del conocimiento de lo útil, a lo útil de conocer**
Junta de la Asociación Acex/Eske, Donostia / San Sebastián

10/23/2017 **Materia. Ciencia. Belleza** III International Encounter on Literatura and Science.
Materia, vida y conciencia desde la ciencia y literatura, Donostia / San Sebastián

11/07/2017 **La sublime utilidad de la ciencia inútil** IV International Congress
"Derecho, filosofía, economía, sociología, psicología y educación en un mundo global. Paz y justicia para una convivencia cultural comunicativa", Santo Domingo

11/07/2017 **Ciencia y belleza** Honoris Causa by P.M. Etxenike
Universidad Autónoma de Santo Domingo

11/09/2017 **De lo pequeño a lo grande... de lo simple a lo complejo**
Academia de Ciencias de la República Dominicana, Santo Domingo

11/23/2017 **Ciencia & belleza** Jakiunde, Aránzazu

Scientific Highlights

Global method for electron correlation

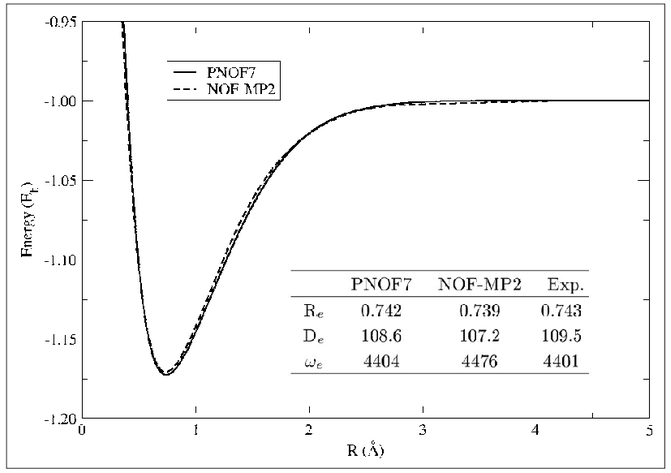
M. Piris
Physical Review Letters 119, 063002 (2017)

This work presents a new single-reference method for capturing static and dynamic electron correlation. The reference is a determinant wavefunction formed with natural orbitals capable of recovering the static correlation. The dynamic correlation is calculated using a modified MP2 theory. Double counting is avoided by introducing the amount of correlation in each orbital as a function of its occupation. The values obtained are in very good agreement with experimental data.

In electronic structure theory, accurate solutions require a balanced treatment of both static and dynamic correlation. Nowadays, it is necessary to resort to multi-reference methods for correctly handling both types of correlation, however, these techniques are often expensive and demand prior knowledge of the system. On the other hand, single-reference correlation methods are well-established for dynamic correlation, but are unsatisfactory for systems with static correlation. In this article, a single-reference method is proposed capable of achieving both dynamic and static correlation even for those difficult cases in which both types of correlation are equally present.

The starting-point is a determinant wavefunction formed with natural orbitals (NOs) obtained from a new interacting-pair model. The latter leads to a natural orbital functional (NOF) named PNOF7 capable of recovering the complete intra-pair, but only the static inter-pair correlation. Using the solution of the NOF, two new energy functionals are defined for both dynamic (E_{dyn}) and static (E_{sta}) correlation. E_{dyn} is derived from a modified second-order Møller-Plesset perturbation theory (MP2), while E_{sta} is obtained from the static component of the PNOF7. Double counting is avoided by introducing the amount of static and dynamic correlation in each orbital as a function of its occupation. The total energy is represented by the sum $E_{hf}+E_{dyn}+E_{sta}$, where E_{hf} is the Hartree-Fock energy obtained with natural orbitals. The resulting working formulas allow for static and dynamic correlation to be achieved in one shot, as is the case in the standard single-reference perturbation theory.

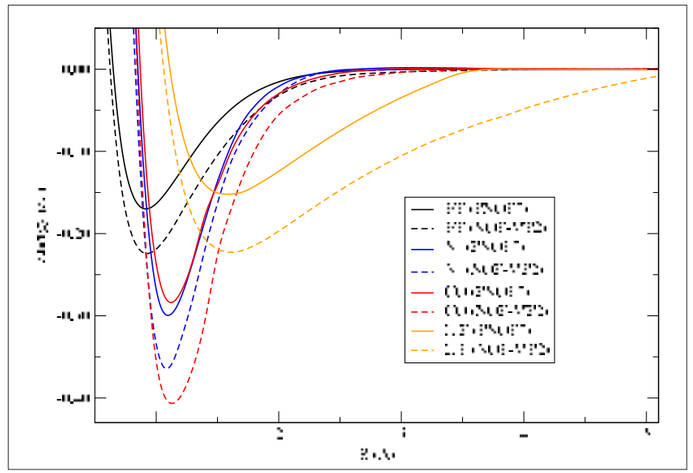
The new procedure called NOF-MP2 is extraordinarily simple and size-consistent, which is essential for applying it to extended systems. It is applied successfully to homolytic dissociation of a selected set of diatomic molecules that encompass very dissimilar interactions ranging from weak to strong bonds, thus sweeping a wide range of correlation regimes. The NOF-MP2 method is not limited to PNOF7 NOs, it can also be used with NOs obtained from other approximation able of recovering static correlation. With efficient approaches, based on recent developments of NOF and MP2 theories, NOF-MP2 could become a valuable tool for treating large systems with hundreds of atoms.



	PNOF7	NOF-MP2	Exp.
R_e	0.742	0.739	0.743
D_e	108.6	107.2	109.5
ω_e	4404	4476	4401

Potential energy curves for the Hydrogen molecule.

The new procedure called NOF-MP2 is extraordinarily simple and size-consistent



Potential energy curves of diatomic molecules that encompass very dissimilar interactions ranging from weak to strong bonds.

Single-reference correlation methods are well-established for dynamic correlation, but are unsatisfactory for systems with static correlation

Riboflavin as a bioorthogonal photocatalyst for the activation of a Pt-IV prodrug

S. Alonso-de Castro, E. Ruggiero, A. Ruiz-de-Angulo, E. Rezabal, J.C. Mareque-Rivas, X. Lopez, F. Lopez-Gallego, and L. Salassa
Chemical Science 8, 4619 (2017)

The combination of catalysis and bioorthogonality promises to have an impact on drug discovery and bioimaging. Bioorthogonality, a term coined by Carolyn R. Bertozzi in 2003, refers to any chemical reaction that can occur inside of living systems without interfering with native biochemical processes. Catalytic turnover can boost the efficiency of bioorthogonal chemical reactions, unveiling new strategies for prodrug activation and uncaging of molecular probes.

This work describes an original photocatalysis approach to control the reactivity of transition metal complexes in a bioorthogonal fashion. In a new type of light-driven reaction, the exogenous biological molecule riboflavin (Rf) functions as a bioorthogonal photocatalyst and a metal complex as unconventional substrate (Figure 1).

Metal complexes are typically regarded as catalysts that convert organic substrates into more valuable compounds; however, to date, catalytic transformations of metal complexes are practically unknown and represent a complete new way of thinking in catalysis. Their development can expand the scope of bioorthogonal chemical reactions to inorganic substances and metal-based prodrugs, fostering the creation of new inorganic chemistry toolkits for biology and medicine.

The photoredox features of riboflavin are crucial in this new type of catalytic process. In fact, riboflavin selectively catalyzes the photoreduction of the Pt^{IV} cisplatin prodrug *cis,cis,trans*-$[Pt(NH_3)_2(Cl)_2(O_2CCH_2CH_2CO_2H)_2]$ in biological environments such as in cell culture media, where numerous chemical and biological species are present and could potentially interfere adversely. Photocatalysis takes place using 460-nm light, a wavelength that is ineffective when directly applied to the PtIV prodrug.

The unusual catalyst/substrate pair enables the selective activation of the Pt^{IV} prodrug with exceptionally low doses of blue light, and induce apoptotic death in PC-3 human prostate cancer cells (Figure 2).

In principle, photocatalysis can help expand the therapeutic potential of platinum prodrugs. Efficient light activation of Pt^{IV} complexes through catalysis may help localize the cytotoxic effects of Pt drugs, increase their dosing at the tumour target, and reduce their systemic toxicity. Riboflavin (vitamin B2) is a highly biocompatible molecule, and its capacity to function in a bioorthogonal fashion may serve to enhance the selectivity of metal-based drugs by minimizing side reactions.

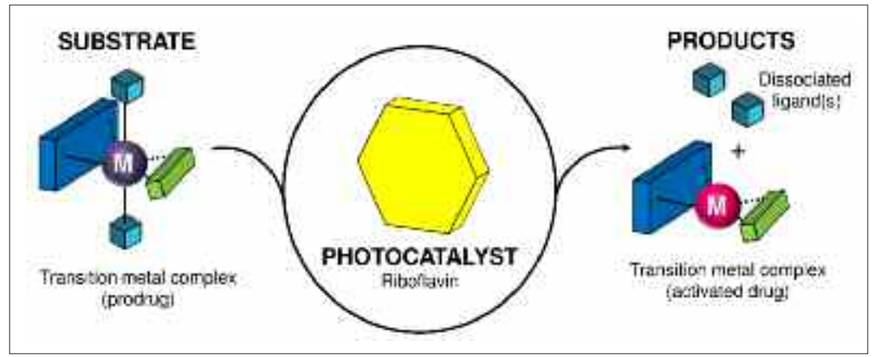


Figure 1. Transition metal complex acting as substrate and its bioorthogonal activation by riboflavin which functions as photocatalyst.

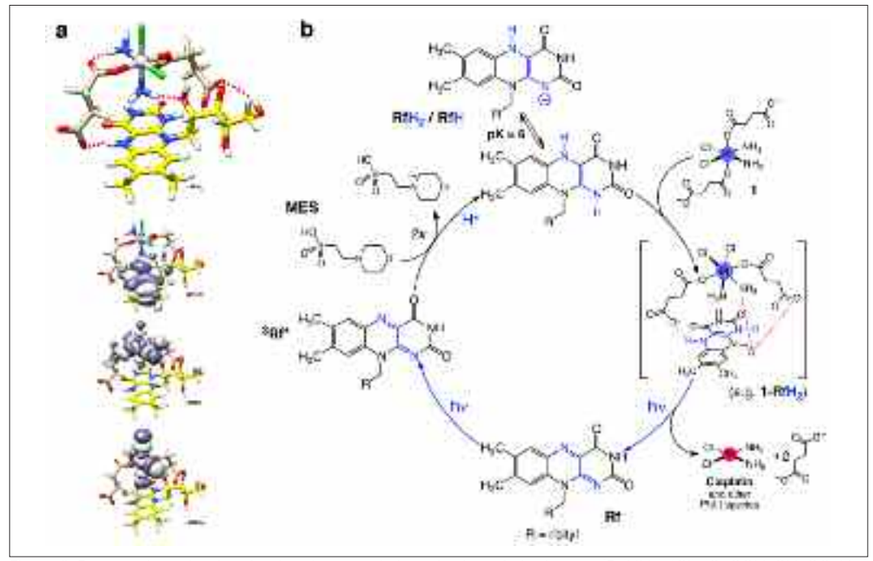


Figure 2. Proposed mechanism for the photocatalytic activation of *cis,cis,trans*-$[Pt(NH_3)_2(Cl)_2(O_2CCH_2CH_2CO_2H)_2]$ by riboflavin. (a) Computed structures and frontier molecular orbitals of a selected riboflavin-Pt^{IV} adduct (1-RfH_2). (b) Riboflavin (Rf) absorbs 460-nm photons to generate the triplet excited state (3Rf*) and eventually liberating cytotoxic Pt^{II} species by regenerating the riboflavin catalyst.

Catalytic transformations of metal complexes are practically unknown and represent a complete new way of thinking in catalysis

Width-dependent band gap in armchair graphene nanoribbons reveals Fermi level pinning on Au(111)

N. Merino-Díez, A. Garcia-Lekue, E. Carbonell-Sanromà, J. Li, M. Corso, L. Colazzo, F. Sedona,
D. Sánchez-Portal, J.I. Pascual, and D.G. de Oteyza
ACS Nano 11, 11661 (2017)

Combining local tunneling spectroscopy and *ab initio* electronic structure calculations, we have investigated the energy level alignment evolution of valence and conduction bands of armchair-oriented graphene nanoribbons (aGNR) on Au(111) as their band gap shrinks with increasing width. Interestingly, valence bands are found to show Fermi level pinning as the band gap decreases below a threshold value, which is of critical importance to understand the properties of potential contacts in GNR-based devices.

Graphene nanoribbons (GNRs) have long been proposed as extremely interesting materials for a variety of applications, e.g. field effect transistors. Interestingly, it has been found that the device performance is strongly dominated by contact effects, in particular, by the Schottky barrier at the GNR–contact interface. However, despite its key role in the ultimate response of such GNR-based devices, a systematic study of the energy level alignment between GNRs and common contact materials is still missing.

In this work, we amend our understanding of such interface energetics between GNRs and gold, in particular, Au(111) surfaces. Armchair-oriented nanoribbons (aGNRs), which are known to display a width-dependent band gap, can be classified into three different subfamilies depending on the number of dimer lines p across their width (3p , 3p+1, or 3p+2), their band gaps being inversely proportional to the width within each of those families. We report a systematic study of the band gap and energy level alignment of GNRs focused on the 3p family, addressing from the smallest possible GNR (3-aGNR) to its four immediately following sister structures (6-, 9-, 12-, and 15-aGNRs). Starting from the synthesis of poly-para -phenylene wires (PPP or 3-aGNR) on Au(111), subsequent annealing drives their lateral fusion and results in the required atomically precise GNRs of varying width. The characterization by scanning tunneling spectroscopy (STS) and density functional theory (DFT) calculations reveals, in addition to the width-dependent band gap, the onset of Fermi level pinning for widths ≥ 6 dimer lines.

In conclusion, we provide spectroscopic evidence of the width dependent band gap predicted for armchair graphene nanoribbons a decade ago and the associated energy level alignment. Most importantly, Fermi level pinning of the valence band is found on wide aGNRs, in qualitative agreement with DFT calculations. Our findings have important implications on the energy level alignment across GNR/metal interfaces, which may in turn be crucial for future GNR-based devices displaying similar interfaces at charge collection electrodes.

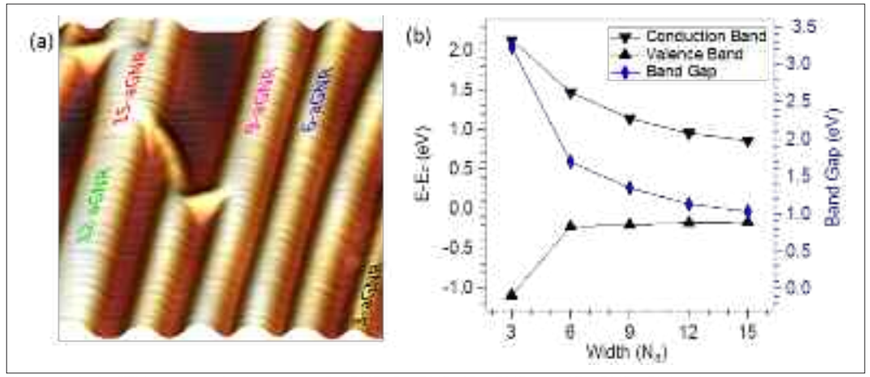


Figure 1. (Left) STM topography image on 6-aGNR, 9-aGNR, 12-aGNR and 15-aGNR. (Right) Average spectroscopic results for valence and conduction bands (black lines, left scale) and the resulting band gaps (blue line, right scale).

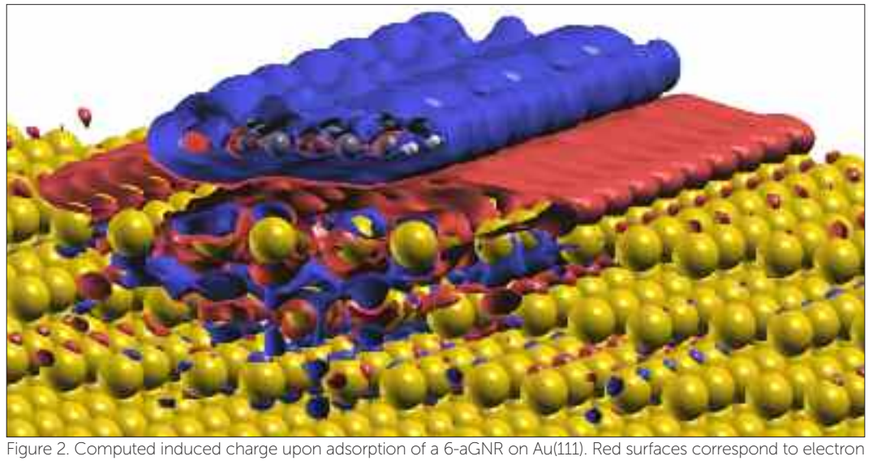


Figure 2. Computed induced charge upon adsorption of a 6-aGNR on Au(111). Red surfaces correspond to electron accumulation, while blue surfaces correspond to electron depletion. Pauli repulsion by the ribbon electrons pushes the electrons of gold towards the surface, giving rise to a modification of the surface dipole with respect to that of extended graphene. The modification will be larger the narrower the ribbon. An accurate determination of the surface dipole is instrumental for determining the alignment of the aGNR levels with respect to the surface.

Valence bands of armchair-oriented graphene nanoribbons on Au(111) are found to show Fermi level pinning as the band gap decreases below a threshold value

Catalysis of a 1,3-dipolar reaction by distorted DNA incorporating a heterobimetallic platinum(II) and copper(II) complex

I. Rivilla I, A. de Cozar, T. Schafer, F.J. Hernandez, A.M. Bittner, A. Eleta-Lopez, A. Aboudzadeh, J.I. Santos, J.I. Miranda, and F.P. Cossio
Chemical Science 8, 7038 (2017)

We all know that the main role of DNA is the storage of genomic information leading to the biosynthesis of proteins via diverse forms of RNA. In turn, proteins play multiple roles in living systems, catalysis being among the most important ones. But recent discoveries add more to the complexity of these molecules: they are also catalysts. Catalytic RNAs are called ribozymes and DNAs, deoxyribozymes. This work focuses on the latter.

Because DNA is structurally less versatile than RNA and proteins, additional molecules and functional groups are required to expand the catalytic space of DNA. The feasibility of this concept by intercalation of aza-chalcones in the double helix and subsequent coordination to copper salts was brilliantly demonstrated by Roelfes and Feringa in 2005.

Despite the relevance of (3 + 2) cycloadditions in the chemical synthesis of five-membered rings, the enzymatic version of this reaction has not been identified in living systems. Only a very recent example of a possible enzymatic 1,3-dipolar reaction has been reported to date. In addition, nonenzymatic 1,3-dipolar reactions have been postulated in the biosynthesis of several alkaloids and natural products.

Now, a team of researchers from UPV/EHU and DIPC, has described the first example of a DNA-assisted 1,3-dipolar reaction in water. It is a biomolecule-assisted (3 + 2) cycloaddition between azomethine ylides and alkenes to produce unnatural proline derivatives. The design of the covalent modification of DNA was based on the ability of Pt(II) chemotherapeutic drugs to bind mainly 1,2-intrastrand GpG units, i.e., regions of DNA where a guanine nucleotide is followed by another guanine nucleotide (GpG is short hand for guanine-phosphate-guanine), thus providing a concave-convex distortion of the double helix that could mimic the active sites of metalloenzymes. In a previous work the researchers had reported that new chiral ligands can bind Cu(II) salts and efficiently catalyze (3 + 2) cycloadditions involving azomethine ylides. They reasoned that a DNA–Pt(II)–Cu(II) heterobimetallic complex similar to that depicted in Figure 1 could catalyze this reaction. Something that was feasible according to computational-modelling calculations.

The results indicate that a suitable bimetallic complex based on Pt(II) can distort the double helix of DNA to generate an active site similar to those found in well-known metalloenzymes. The proposed reaction mechanism, based on quantum mechanical calculations, is compatible with thermally allowed mechanisms leading to the exclusive formation of racemic endo-cycloadducts.

This work demonstrates that modified biomolecules can catalyse chemical reactions in water, for which there is no equivalent in living systems.

A suitable bimetallic complex based on Pt(II) can distort the double helix of DNA to generate an active site similar to those found in well-known metalloenzymes

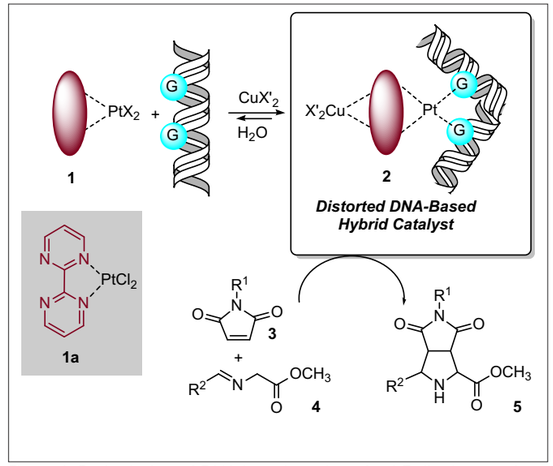


Figure 1. Basic design of DNA-based catalysts for 1,3-dipolar reactions. The distortion of DNA by coordination of G bases with Pt(II) is shown.

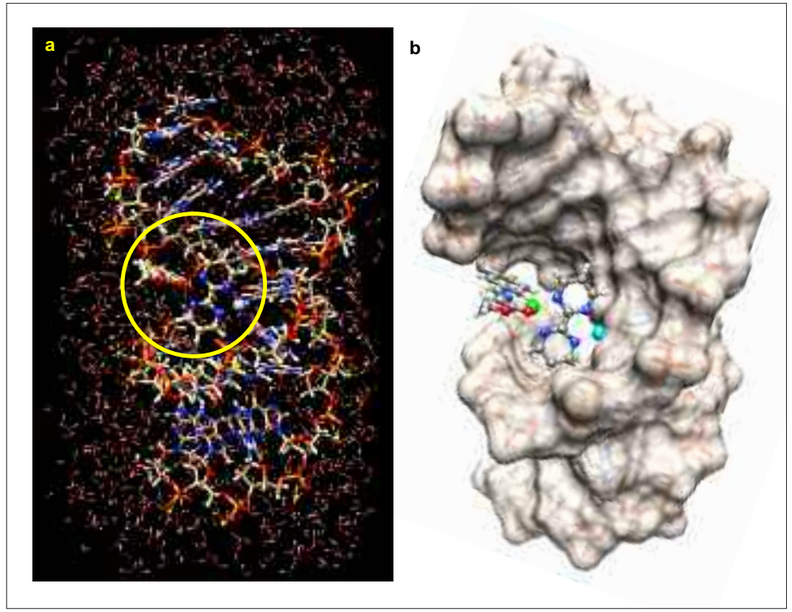


Figure 2. (a) Fully optimized structure of a DNA double strand containing the d(CCTCTG*G*TCTCC)-d(GGAGACCAGAGG) sequence. (b) (b) The same optimized structure but showing the solvent Pt(II) and Cu(II) atoms are represented in light blue and green, respectively.accessible surface of the DNA fragment.

Theoretical insights into unexpected molecular core level shifts: chemical and surface effects

A. Sarasola, M. Abadía, C. Rogero, and A. Garcia-Lekue
Journal of Physical Chemistry Letters 8, 5718 (2017)

A set of *ab initio* tools are employed to elucidate the influence of chemical and surface-induced changes on the core level shifts of X-ray photoelectron spectroscopy experiments. We address surface induced effects, such as splitting of the lowest unoccupied molecular orbital or local electrostatic effects, demonstrating that these cannot account for the unexpected huge core level shifts often measured experimentally. Our calculations also demonstrate that molecular hydrogenation is an alternative explanation for the appearance of such extra peaks in the XPS spectra. More importantly, it is anticipated that this hydrogenation reaction will occur in many UHV experiments where the molecular evaporation is performed at low temperatures.

Advances in scientific knowledge and technological tools achieved over the last decades, have been aimed at the development of bioinspired nanodevices. Covering an inorganic substrate with organic matter is an appropriate and viable architecture for such devices. The X-ray Photoelectron Spectroscopy (XPS) technique and, in particular, the measurement of the shifts in the binding energy of different core levels, make it possible to verify the chemical integrity of a molecule, to identify changes in its composition and to sense the changes in the local electrostatic environment. However, disentangling the collective electrostatic effects from the chemical shifts is not straightforward and it results crucial for a correct interpretation of experimental XPS spectra.

A team of researchers from DIPC and CFM has carried out the first exhaustive theoretical study of the origin of unexpected signals in the XPS spectra of molecule-substrate complexes. Using a set of density-functional theory (DFT) based tools, they have determined the distinct influence that chemical changes or surface-induced effects might have on the molecular core level shifts of phthalocyanine molecules deposited on Cu(110). As shown in Figure, the N1s spectra recorded with the substrate at 210K reveal an unpredicted double peak structure, which is not observed when the molecules are deposited on the substrate at RT. Besides, it has been demonstrated that such extra peaks in XPS spectra are likely to be originated by the hydrogenation of the molecules due to the capture of residual hydrogen (Figure 2). Calculations, therefore, exclude LUMO splitting, surface effects and molecular demetalation as possible origins of the double peak detected in the low coverage and low temperature N 1s core level spectra.

To conclude, the findings reported here might clarify a few of the uncertainties in the measured electronic properties of organic molecules on surfaces, which represents an important advancement towards the ability to tune the functionalities of molecular complexes and delivers important input for the development of nanoelectronic devices based on organic molecules.

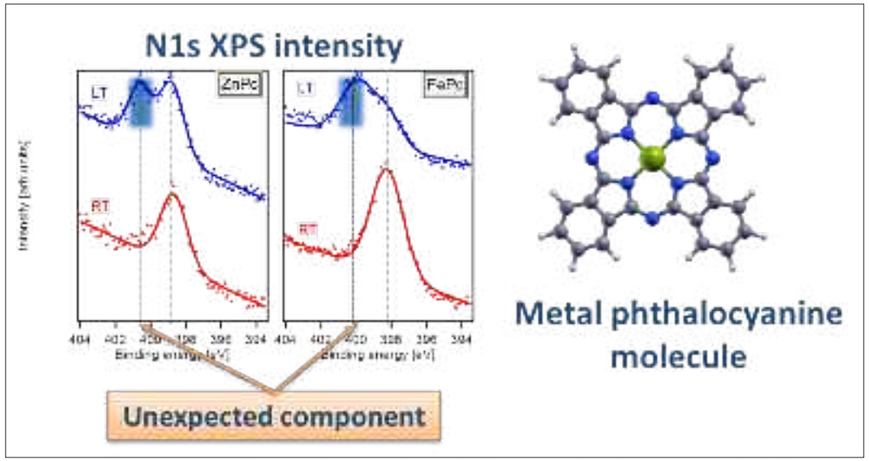


Figure 1. Experimental N 1s XPS spectra for 1 ML of ZnPc (left) and FePc (right) deposited on Cu(110) with the substrate at RT and at 210K (LT).

A team of researchers from DIPC and CFM has carried out the first exhaustive theoretical study of the origin of unexpected signals in the XPS spectra of molecule-substrate complexes

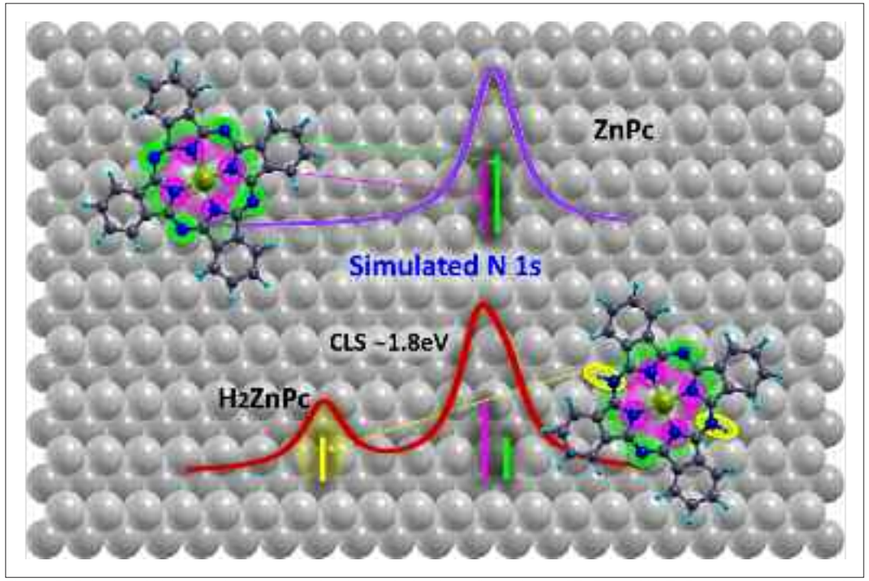


Figure 2. Calculated N 1s core level spectra for the optimized configurations of ZnPc and H_2ZnPc deposited on Cu(110).

DIPC HIGHLIGHT 2017

The role of the topological constraints in the chain dynamics in all-polymer nanocomposites

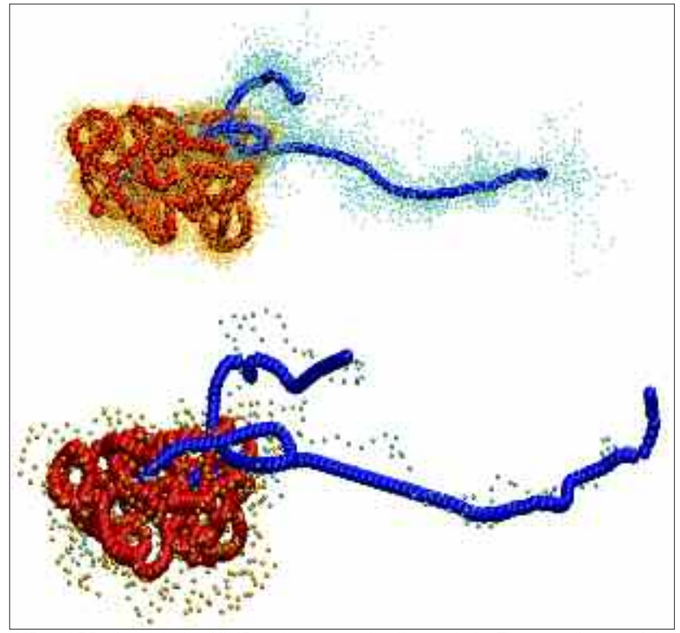
P. Bacova, F. Lo Verso, A. Arbe, J. Colmenero, J.A. Pomposo, and A.J. Moreno
Macromolecules 50, 1719-1731 (2017)

The specific architecture of the soft nanoparticles in all-polymer nanocomposites plays a key role on the entanglements experienced by the linear matrix, which are at the origin of the viscoelastic properties of the system.

In a long-lasting effort to get a good compatibility between the nanoparticles and the linear polymer matrix, all-polymer nanocomposites are gaining increasing attention. The presence of soft penetrable polymer nanoparticles in such systems is expected to affect the fundamental topological constraints (entanglements) that originate from chain uncrossability and that control the viscoelastic properties of the system. In this pioneering computational study of all-polymer nanocomposites, we shed light on this question by discussing simulations in the framework of the tube model.

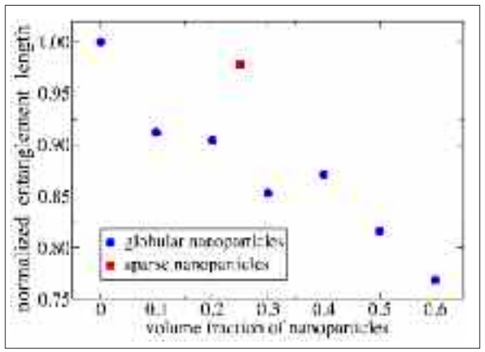
We investigate all-polymer nanocomposites, formed by strongly entangled linear chains and single-chain polymer nanoparticles (SCNPs), by means of large-scale simulations. SCNPs are soft nano-objetcs obtained through intramolecular cross-linking of linear chains, with potential applications as nanocarriers, catalytic or rheological agents, among others. To distinguish the role of the soft penetrable character of the SCNPs in the topological constraints from other specific contributions present in experiments, the simulations are performed at constant density and with identical segmental mobility and monomer excluded volume for the SCNPs and the linear chains. Every composition leads to a well-dispersed nanocomposite with fully penetrated nanofillers. Hence, unlike in the case of composites with hard nanofillers, the SCNPs do not exert confinement effects on the linear chains and only contribute to the topological constraints.

We determine the entanglement length of the linear chains by analyzing their tube paths as a function of the concentration and topology of the SCNPs. The tube path is characterized through the isoconfigurational mean path (IMP) and the primitive path (PP) (see figure). In the analysis we use different estimators proposed in the literature. The IMP and PP analysis in the nanocomposites with sparse SCNPs yields values of the entanglement length smaller and larger, respectively, than in the reference pure linear melt, though small variations are observed. A more consistent trend is found in the nanocomposites with globular SCNPs, where both the IMP and PP analysis unambiguously reveal that the linear chains are more entangled than in the pure linear melt ("tube narrowing"). Such differences between the effects of SCNPs with different topologies are presumably related to the much higher fraction of threadable loops present in the globular SCNPs, with respect to their sparse counterparts, which effectively lead to more topological constraints.



IMP and PP of a globular SCNP and a penetrating linear chain. The coordinates of the red (SCNP) and blue (chain) monomers are obtained after applying the IMP procedure (top panel) and the PP construction (bottom panel). The coordinates of the real configurations used for such constructions are drawn as yellow (SCNP) and cyan dots (chain).

We determine the entanglement length of the linear chains by analyzing their tube paths as a function of the concentration and topology of the single-chain polymer nanoparticles



Entanglement length of the linear chains, normalized by the value of the homopolymer, as a function of the nanoparticle volume fraction. Circles and squares are data obtained from IMP analysis for nanocomposites with globular and sparse nanoparticles, respectively.

DIPC HIGHLIGHT 2017

Topological quantum chemistry

B. Bradlyn, L. Elcoro, J. Cano, M.G. Vergniory, Z. Wang, C. Felser, M. I. Aroyo, and B.A. Bernevig
Nature 547, 298 (2017)

In this work we propose a complete electronic band theory, which builds on the conventional band theory of electrons, highlighting the link between the topology and local chemical bonding. This theory of topological quantum chemistry provides a way to cassify the possible band structures that arise from local atomic orbitals, and to show which are topologically non-trivial. Our electronic band theory sheds new light on known topological insulators, and can be used to predict many more.

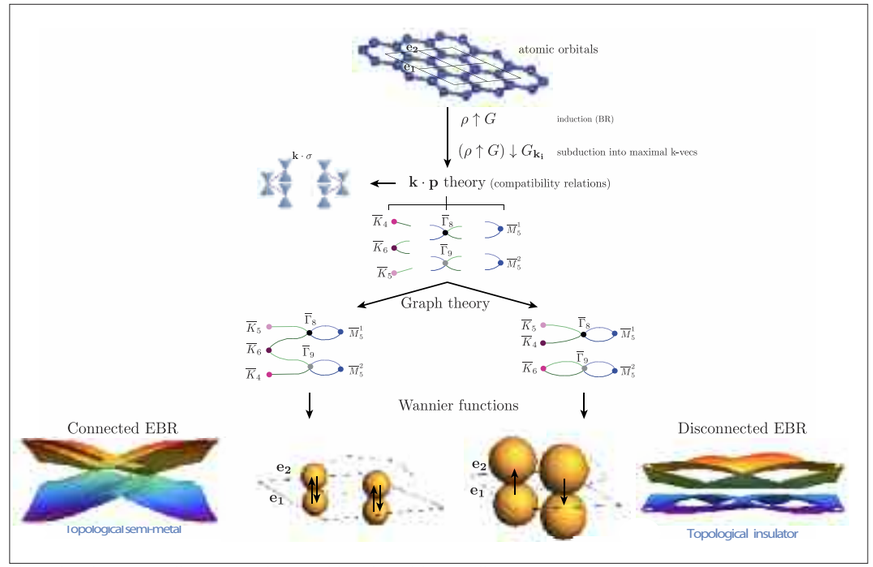
Topological materials, which hold promise for a wide range of technological applications due to their exotic electronic properties, have attracted a great deal of theoretical and experimental interest over the past decade, culminating in the 2016 Nobel Prize in physics. The materials` electronic properties include the ability of current to flow without resistance and to respond in unconventional ways to electric and magnetic fields.

Until now, however, the discovery of new topological materials occurred mainly by trial and error. This new approach allows researchers to identify a large series of potential new topological insulators, based on band theory. In this work the researchers first compiled all the possible ways energy bands in a solid can be connected throughout the Brillouin zone to obtain all realizable band structures in all non-magnetic space-groups. Group theory itself places constraints – "compatibility relations" – on how this can be done. Each solution to these compatibility relations gives groups of bands with different connectivities, corresponding to different physically-realizable phases of matter (trivial or topological). The scientists solve all compatibility relations for all 230 space groups by mapping connectivity in band theory to the graph-theoretic problem of constructing multipartite graphs. Then the researchers developed the tools to compute how the real-space orbitals in a material determine the symmetry character of the electronic bands. Given only the Wyckoff positionsand the orbital symmetry (s, p, d) of the elements/orbitals in a material, they derive s the notion of band representation (all bands linked to localized orbitals respecting the crystal symmetry), to the physically relevant case of materials with spin-orbit coupling and/or time-reversal symmetry, and identify a set of elementary band representations (EBR). These elementary band representations allow to easily identify candidate semimetallic materials: If the number of electrons is a fraction of the number of connected bands forming an elementary band representation, then the system is a symmetry-enforced semimetal. If, however, the number of connected bands is smaller than the total number of bands in the elementary band representation, then the disconnected bands are topological. Thus, the researchers have provided a full classification of all topological crystalline insulators. And they show how powerful the method is by predicting hundreds of new topological insulators and semimetals.

Cover image: JVG

This new approach allows researchers to identify a large series of potential new topological insulators, based on band theory

This work appeared on the cover of *Nature* and as the editor put it: "[...] a new and complete theory for calculating the topological properties of the electronic band structures of materials. [...] As a result, they complete the theory of electronic band structure [...] The theory should greatly simplify the search for further materials with exotic properties and also shed light on the underlying physics of existing topological materials."



How the theory applies to graphene with spin-orbit coupling.

Angular momentum induced delays in solid state photoemission enhanced by intra-atomic interactions

F. Siek, S. Neb, P. Bartz, M. Hensen, C. Strüber, S. Fiechter, M. Torrent-Sucarrat, V.M. Silkin, E.E. Krasovskii, N.M. Kabachnik, S. Fritzsche, R. Díez Muiño, P.M. Echenique, A.K. Kazansky, N. Müller, W. Pfeiffer, and U. Heinzmann
Science 357, 1274 (2017)

Even more than 100 years after Einstein's explanation of photoemission the process of electron emission from a solid material upon illumination with light still poses challenging surprises. Here, ultrashort pulses of light were employed to start a race between electrons photoemitted from different initial states in a solid. Timing this race reveals an unexpected result: The fastest electrons arrive in last place.

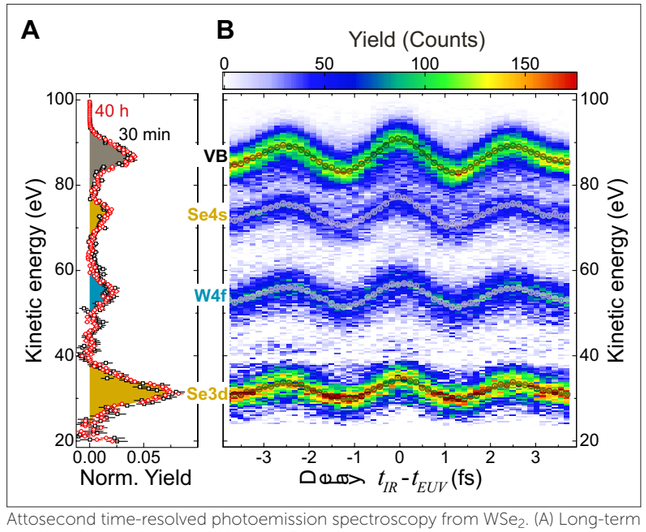
The explanation of the photoelectric effect was the major work cited in the award to Albert Einstein of the Nobel Prize in Physics in 1921. After more than a century of theoretical, experimental, and commercial development, we could assume that we knew everything there was to be known about the photoelectric effect. Not so. In a combined experimental and theoretical effort, researchers from different German institutions, UPV/EHU, CFM, and DIPC showed in this work that the process is not correctly captured in common models of solid-state photoemission. Based on attosecond time-resolved photoemission spectroscopy, the authors show that the motion of a photoemitted electron is strongly affected by interactions inside the atom from which the electron is emitted. Electrons photoemitted from a surface remain trapped for a while, dynamically confined by the centrifugal barrier around the atoms. The motion of these electrons around the nuclei, before being eventually emitted, is kind of a dance leading to an intuitive picture that the electrons that remain longer dancing around the atom lose the race and are emitted last. In contrast, electrons going straight win the race.

Experimentally resolving the tiny delays in the photoemission process required timing the emission event, i.e. the moment when the electron leaves the material, with an unprecedented resolution of 10^{-17} seconds. The choice of tungsten diselenide (WSe_2) as material turned out to be essential. WSe_2 yields a photoemission spectrum dominated by four emission channels with different electronic initial-state characteristics. According to standard models, all these electrons should be emitted at once, but that is not what is observed: there are relative emission delays.

Quantitative theoretical modelling of the intra-atomic processes and the electron propagation in the semiconductor crystal demonstrated that the initial orbiting motion shall not be neglected if the dynamics of the photoemission process from a solid is considered. The researchers reached the conclusion that the delays between the four photoemission channels can only be explained by accounting for both propagation and intra-atomic delays. The intra-atomic delays depend on the angular momentum of the initial localized state and are determined by intra-atomic interactions. Once intra-atomic electron-electron interaction and angular momentum of the initial localized state are incorporated into the model for WSe_2, there is a remarkable agreement between theory and experiment.

The reported advances in understanding photoemission from solids became feasible based on recently developed attosecond laser techniques. Control of light with attosecond (10^{-18} second) resolution opens fascinating views on electron dynamics on the atomic scale.

Left: An artist's rendition of the intra-atomic mechanism for which the photoemission of some electrons is relatively delayed: They remain trapped for a while, dynamically confined by the centrifugal barrier around the atoms. The motion of these electrons around the nuclei, before being eventually emitted, is kind of a dance.



Attosecond time-resolved photoemission spectroscopy from WSe_2. (A) Long-term stability of the surface over 40 hours. Background-corrected photoemission spectra recorded 30 min (black circles) and 40 hours (red circles) after cleaving. The photoelectron peaks for VB, Se 4s,W 4f, and Se 3d are indicated. The spectra are normalized to the total yield after background subtraction. (B) Streaking spectrogram. As a function of the delay between the IR and EUV pulses, the photoemission spectra (after background subtraction) are shown as a density plot. For each delay, the energy positions (overlaid symbols) of the VB, Se 4s, W 4f, and Se 3d emissions and the corresponding simultaneously fitted IR field-time dependence yielding the delay parameters Dt for each emission channel (continuous overlaid lines) are shown.

Attosecond-scale processes are strong tests for theoretical models of solid-state photoemission

Controlled spin switching in a metallocene molecular junction

M. Ormaza, P. Abufager, B. Verlhac, N. Bachellier, M.-L. Bocquet, N. Lorente, and L. Limot
Nature Communications 8, 1974 (2017)

In this work we change the effective spin of a single molecule by modifying the molecule/metal interface in a controlled way using a low-temperature scanning tunneling microscope: A nickelocene molecule reversibly switches from a spin 1 to 1/2 when varying the electrode–electrode distance from tunnel to contact regime. This switching is experimentally evidenced by inelastic and elastic spin-flip mechanisms observed in reproducible conductance measurements and understood using first principle calculations. Our work demonstrates the active control over the spin state of single molecule devices through interface manipulation.

Nickelocene molecules consists of two carbon pentagon-rings (cyclopentadienyl) sandwiching a nickel atom. Nickel contains 8 electrons placed in d-electrons. The molecule has a spin of 1 corresponding to two unpaired electrons in the d-shell of the Nickel atom. This is clearly seen in scanning tunneling microscope (STM) measurements where the differential conductance is recorded. The differential conductance is proportional to the number of possible "paths" a transmitting electron undertakes between substrate and tip. If the electron can yield part of its energy to other degrees of freedom of the system, new paths open and the conductance increases. This is the case for the present molecule, when the applied voltage is larger than ~5 mV. This bias corresponds to the energy of turning the molecule spin (S=1) by 90 degrees, and it is due to the intrinsic magnetic anisotropy of the molecule. The measured differential conductance reflects a large change in conductance at this threshold. Everything is consisting with what we know from the molecule and STM studies.

However, when the free electrode of the STM (the tip) is pressed against the molecule, the steps abruptly disappear and a peak at zero bias appears. Figure 1 shows the conductance in this contact regime (a), compared to the previous tunneling regime (b). Two shocking experimental facts: a zero bias peak appears of nowhere and the change is extremely abrupt, it is sufficient to move the tip by 0.1 Angström to see this change. Calculations using DFT with two electrodes pressing a Nickelocene molecule (Figure 2) show that there is a change in the spin of the molecule. When the electrodes are pressing, the spin is ½. Then the peak at zero bias would be consistent with a Kondo peak caused by the random flipping of the molecular spin under interaction with electrons from the electrode. And the calculations show that the change in spin is very fast.

Moreover, our calculation tells us the mechanism. As the electrodes close on the molecule, the enviromental electronic density is very much enhanced. As a consequence, the direct Coulomb repulsion between two electrons in the molecules gets screened by the electrodes. Less repulsion leads to a larger population of the d-shell. Basically, the nicke atom gets one more electron reducing its spin by Hund's rule.

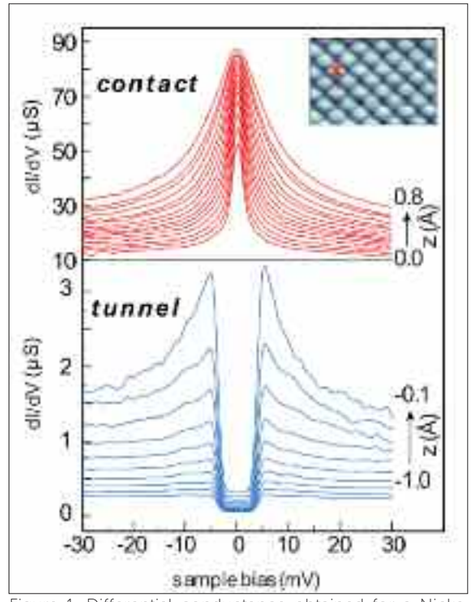


Figure 1. Differential conductance obtained for a Nickelocene molecule when the two electrodes are pressing the molecule (a) and when they are in the tunneling regime (b). There is a clear change of conductance features signaling a change in the spin of the molecule from ½ at contact to 1 in the tunneling regime.

We can reversibly switch the spin of a nickelocene molecule from 1 to 1/2 by varying the electrode–electrode distance from tunnel to contact regime

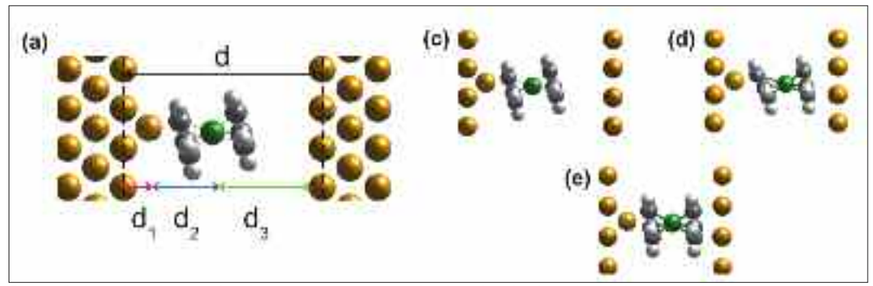


Figure 2. Atomic schemes for the systems computed using density functional theory. (a) is the setup depicting the molecule (Nickelocene, green is the Ni atom, grey the C atoms and white the H atoms, the two cyclopentadienyls are pentagonal rings) and the copper substrate and the tip. The experiments clearly show a poorly coordinated molecule with the tip, then we use a Cu adsorbate to induce a lower coordination with the molecule. The substrate is just a flat Cu (100) surface. (c), (d) and (e) show the changes in molecular arrangement as the electrodes are pressed together.

Extracting chemical information from surface-enhanced Raman spectroscopy

K.-Q. Lin, J. Yi, J.-H. Zhong, S. Hu, B.-J. Liu, J.-Y. Liu, C. Zong, Z.-C. Lei, X. Wang, J. Aizpurua, R. Esteban, and B. Ren
Nature Communications 8, 14891 (2017)

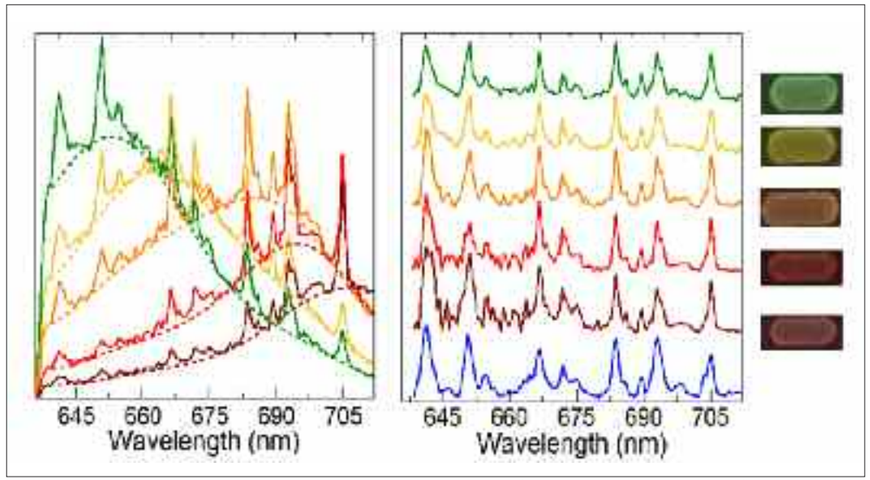
Plasmonic resonances can strongly enhance the strength of the Raman signal emitted by molecules, a considerable advantage for applications that aim at detecting ultra-small quantities. At the same time, however, the plasmon can also distort the signal and thus hide some of the chemical information. This work studies how the photoluminescence signal can be exploited to recover this information.

A main objective in molecular sensing is to extract as much chemical information from as few molecules as possible, not only to identify them but also to learn about their local temperature, orientation, changes on chemical properties, etcetera. In Raman spectroscopy, the information is extracted from the exchange of energy between incoming photons and molecular vibrations. In this way, the vibrational modes can be identified as molecular fingerprints, with all the very rich chemical information that they reveal.

The main drawback of this Raman process is its weak efficiency, which requires significant amounts of molecules to provide a measurable signal. Fortunately, this obstacle can be overcome by using metallic nanoantennas, which interact very efficiently with nearby molecules due the presence of optical plasmonic resonances that strongly confine the optical energy in their proximity. The resulting technique is called Surfaced Enhanced Raman Spectroscopy (SERS) and allows for identifying single molecules.

While SERS has been extraordinarily successful, it does introduce some significant challenges. Notably, each molecular vibration is manifested as a narrow peak in the Raman spectra, and the relative height of these peaks contain significant information. SERS, however, enhances the vibrational peaks with different scalings, which usually does not hinder the identification of the molecules but can lead to extracting misleading information, such as a completely wrong temperature of the molecules.

The main result of the work is to propose a method to recover the real vibrational information compromised in the spectra by focusing on the analysis of the background of the signal emitted by the plasmonic particle. This background is typically ignored; however, by analyzing its physical origin as a photoluminescence process from the metal, and by comparing the theoretical expectation with the careful measurements by collaborators in Xiamen, it is shown that the emission spectral shape contains the necessary information to rescale and largely retrieve the original Raman spectra. This technique should thus represent a significant step towards recovering chemical information in a reliable manner with down to single-molecule sensitivity.



As the aspect ratio of the plasmonic nanoantennas is increased (right images, top to bottom) the plasmonic resonances are redshifted, leading to changes on the relative strength of the Raman peaks (left spectra, with increasing aspect ratio from green to brown). After applying the procedure discussed in the paper, we recover spectra characterized by very similar strength of the relative peaks for all plasmonic structures (right spectra, green to brown) and for a metal surface (blue surface)

We propose a method to recover the real vibrational information compromised in the spectra by focusing on the analysis of the background of the signal emitted by the plasmonic particle

Electronic stopping of slow protons in transition and rare earth metals: breakdown of the free electron gas concept

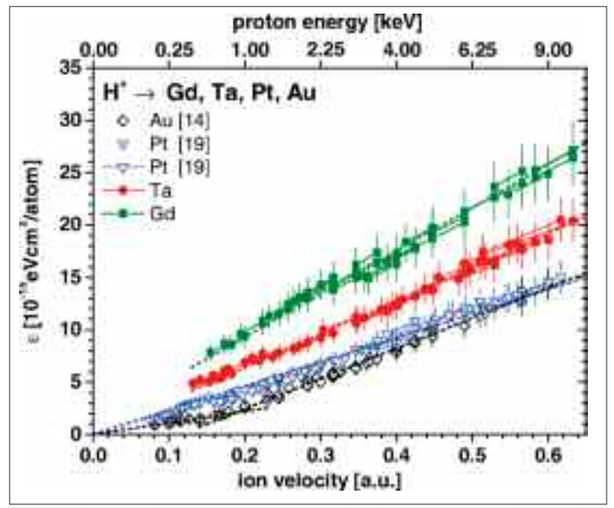
D. Roth, B. Bruckner, M.V. Moro, S. Gruber, D. Goebl, J. I. Juaristi, M. Alducin, R. Steinberger, J. Duchoslav, D. Primetzhofer, and P. Bauer
Physical Review Letters 118, 103401 (2017)

The electronic stopping cross sections (SCS) of Ta and Gd for slow protons have been investigated experimentally. The data are compared to the results for Pt and Au to learn how electronic stopping in transition and rare earth metals correlates with features of the electronic band structures. The extraordinarily high SCS observed for protons in Ta and Gd cannot be understood in terms of a free electron gas model. By calculating the electronic density of states, it was shown that the measured high SCS for Gd and Ta are linked to the high density of unoccupied electronic states above the Fermi level in these metals.

When ions propagate in matter, they are decelerated due to interaction with both nuclei and electrons or in other words, by nuclear and electronic stopping power, respectively. For ion velocities lower than the Fermi velocity of the metal electrons, the electronic energy loss is predominantly due to interaction with valence electrons. For many different kind of metallic targets, it has been shown that the free electron gas (FEG) model represents an adequate approximation to obtain the electronic stopping power in this velocity regime, provided the potential induced by the projectile is calculated within density functional theory.

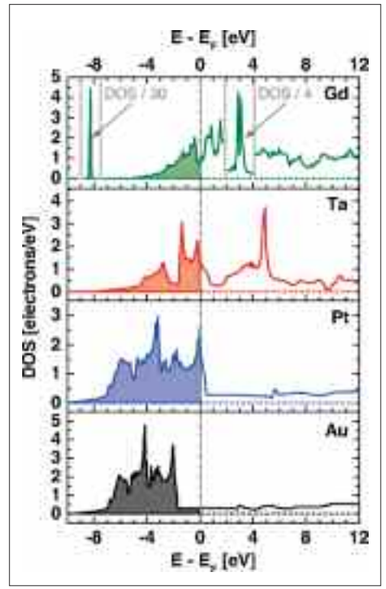
In the present work, experimental measurements of the energy loss of protons traveling at low velocities through Gd, Ta, Pt and Au targets were presented. It was observed that the electronic SCS of both Gd and Ta are considerably higher than that of Pt and Au. Actually, whereas the FEG model explains successfully the stopping power values of Pt and Au in terms of their valence electron densities, it fails completely for Gd and Ta. In fact, it will require to assume absurdly high valence electronic densities to fit the experimental results to those provided by the FEG for these two metals.

By calculating the electronic density of states (DOS) it was shown that the main difference is that, in contrast to Au and Pt, both Gd and Ta present a very high DOS for unoccupied states close to the Fermi energy (EF). As a consequence, the large measured SCS for protons in these metals was linked to the high DOS below and above E_F that allows for low energy excitations with high probabilities. For this reason, it was concluded that the FEG model for the electronic stopping power of slow ions is expected to fail for transition an rare earth metals featuring a high DOS below and above E_F. An adequate description of the problem in these cases will require elaborated many-body theoretical models like, for instance, time dependent density functional theory.



Measured electronic SCS of Au, Pt, Ta, and Gd for protons are displayed as function of the ion velocity in atomic units. The upper abscissa denotes the corresponding proton energies.

The extraordinarily high stopping cross sections observed for protons in Ta and Gd cannot be understood in terms of a free electron gas model



Electronic densities of states (DOS) are shown for the conduction bands of Au, Pt, Ta, and Gd, as function of E-EF. The filled part of the DOS corresponds to the occupied states. For the DOS of Gd dotted lines indicate below and above EF the energy intervals, in which the high features due to the f band were scaled down by factors of 30 and 4, respectively.

Tautomerization of an organic adsorbate driven by non-adiabatic and anharmonic effects

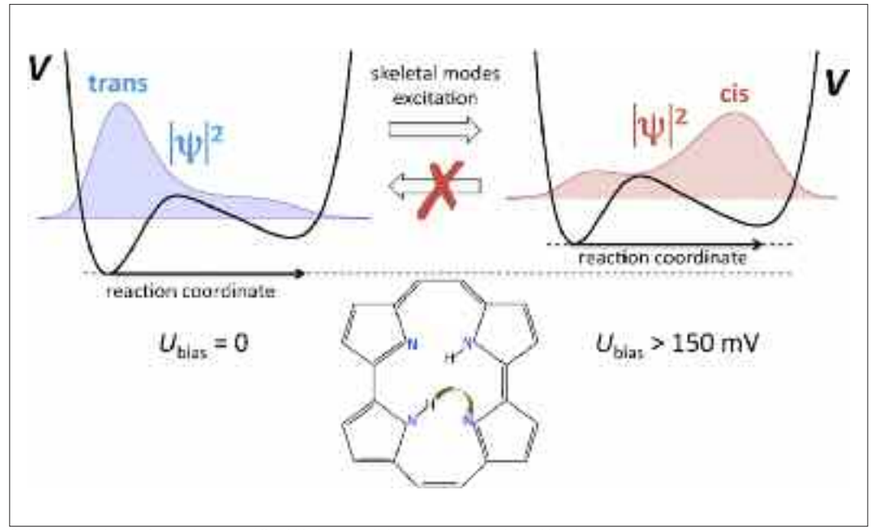
D. Novko, M. Blanco-Rey, and J.C. Tremblay
Journal of Physical Chemistry Letters 8, 1053 (2017)

This letter proposes a model for chemical reactions driven by electrons injected by a STM tip. The variables are mapped onto a one-dimensional problem, accounting effectively for the inelastically scattered electron current (non-adiabaticity) and for the couplings between molecule vibrations (anharmonicity).

Indirect adsorbate transformation by hot electrons has gained prominence as a tool to control the reactivity of species in the condensed phase. In this context, tautomerization of organic molecules, i.e. intramolecular relocation of a light atom, is attractive. Since large changes in reactivity and photochemical properties are associated to tautomerization, much effort is devoted to harnessing its potential in molecular switches. Modern surface science techniques are useful for this purpose, as they allow reaction control at the single-molecule level by means of femtosecond lasers and scanning tunnelling microscopy (STM).

Recently, the Kumagai group (Berlin) reported tautomerization of porphycene (the most stable and highest symmetrical isomer of porphin) on Cu(111) by injection of electrons with a STM tip. The process breaks a NH bond in the molecule cavity and forms a new one in a neighboring N site, while the outer large aromatic ring apparently remains as a spectator. Interestingly, the reaction happens above a STM threshold voltage lower than the NH stretching mode frequency, it can occur tens of nanometers away from the tip position, and it is irreversible at low temperatures.

D. Novko (DIPC), M. Blanco-Rey (UPV/EHU, DIPC), and J.C. Tremblay (FU-Berlin) undertook the challenge of simultaneously explaining all those observations. They have developed a general microscopic quantum-dynamical model based on density functional theory (DFT) that circumvents the need for high-dimensional dynamics. The reaction results from non-adiabatic coupling (NAC) of inelastically scattered electrons/holes and molecule vibrations. However, it cannot be described by existing non-adiabatic models, due to the large number of non-negligibly coupled vibrational modes: here the so-called skeletal modes (wide vibrational spectrum of the aromatic ring) are key. These are common limitations of organic molecular adsorbate manipulation.



Schematic view of porphycene/Cu(111) irreversible tautomerization. Abscisas represent the reaction coordinate (N-H stretch) where the skeletal modes are mapped, deforming the potential as they are excited. At a given threshold voltage, the deformation prompts the reaction.

We have developed a general microscopic quantum-dynamical model based on density functional theory (DFT) that circumvents the need for high-dimensional dynamics

First the NAC-induced anharmonic (de)excitation rates of individual modes are calculated. Then, intermode coupling is treated as a deformation of the adiabatic potential energy curve associated to the N-H bond stretch, i.e. the procedure maps the high-dimensional problem effectively onto a one-dimensional one. All the model quantities are calculated from DFT, ensuring an accurate description of the molecule-substrate van der Waals interaction.

Strong magneto-optical response of nonmagnetic organic materials coupled to plasmonic nanostructures

D. Melnikau, A.A. Govyadinov, A. Sánchez-Iglesias, M. Grzelczak, L. Liz-Marzan, and Y. Rakovich
Nano Letters 17, 1808-1813 (2017)

Plasmonic nanoparticles can significantly modify the optical properties of nearby organic molecules and thus present an attractive opportunity for sensing applications. In this paper, authors show that nonmagnetic organic molecules may exhibit magneto-optical response due to binding to a plasmonic nanoparticle.

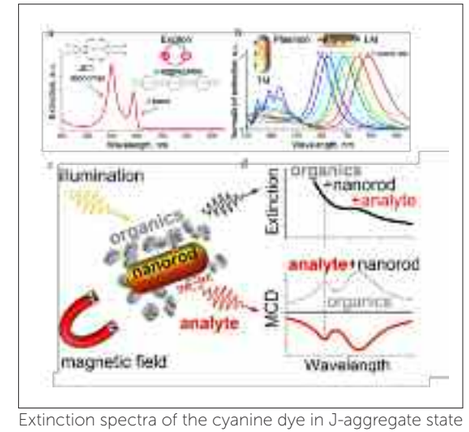
Methods based on magneto-optical (MO) activity measurements, such as magnetic circular dichroism (MCD) spectroscopy and magneto-optic Kerr effect (MOKE), take an important place in the battery of tools for materials. However, direct MCD or MOKE measurements are rarely utilized in biosciences due to the usually very low magneto-optical response of biomolecules. Instead, magnetic methods for chemo- and biosensing typically rely on magneto-plasmonic effects, such as the high MO activity exhibited by plasmonic nanoparticles near their localized surface plasmon resonance. From other hand the utilization of plasmonic nanoarticles in sensing based on conventional absorption, fluorescence, or Raman spectroscopy techniques is often ineffective due to strong absorption background and light scattering, particularly in the case of turbid solutions, cell suspensions, and biological tissues.

Recently we demonstrated that the MO activity of an organic compound itself can be greatly enhanced by coupling to a resonant plasmonic nanoparticle. Specifically, we show that supramolecular J-aggregates (a good model system for assemblies in biological complexes) linked to core–shell Au@Ag nanorods produce strong MCD signal when the resonance of the plasmonic nanoparticles is tuned to the excitonic band of the aggregates, while exhibiting no MCD upon detuning.

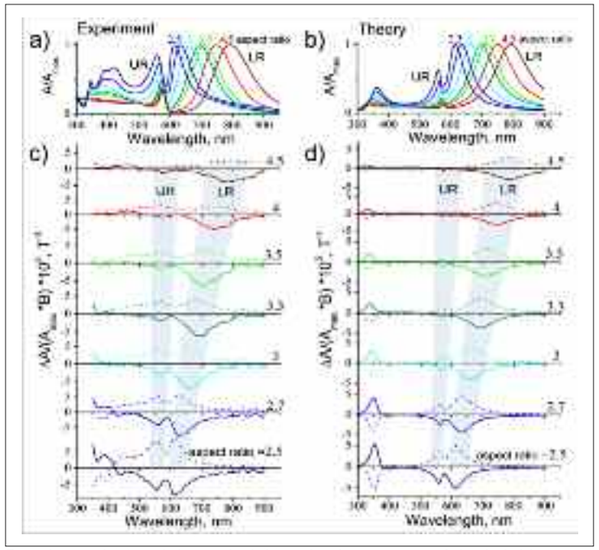
We explained such an enhancement of the MO activity by strong coupling of the J-band exciton and the nanoparticle plasmon and fully support our experimental findings by theoretical modeling. Strong-field confinement around the nanoparticle selectively enhances the MO activity only in those molecules that are bound to the particle surface.

Our findings are fully corroborated by theoretical modeling. Moreover the near-complete absence of MO background from other molecular components could allow for the molecule detection even in the case of strong absorption background or light scattering. Thus, our work creates a new paradigm in sensing, which can make a large impact in materials science, medicine, biology, and pharmacology.

The magneto-optical activity of an organic compound itself can be greatly enhanced by coupling to a resonant plasmonic nanoparticle



Extinction spectra of the cyanine dye in J-aggregate state (a) and bare core–shell Au@Ag nanorods of varying aspect ratios (solid lines), overlaid with theoretical predictions (dashed lines) (b). Panels c) and d) show sketch of hybrid organic-inorganic system and corresponding extinction and MCD spectra.



Experimental (a) and theoretical (b) extinction spectra of the hybrid system of J-aggregates and core–shell Au@Ag nanorods for different aspect ratios. Experimental (c) and theoretical (d) MCD spectra measured under the applied magnetic fields of B = ±1T.

Nonlocal signatures in electronic spin and charge transport in two-dimensional materials

C.L. Huang , Y.D. Chong, and M.A. Cazalilla
Physical Review Letters 119, 136804 (2017)

In this work we uncover two anomalous features in the nonlocal transport behavior of two-dimensional metallic materials with spin-orbit coupling. The observed effects can be used to identify the relative contributions of different spin-charge conversion mechanisms. They should be observable in adatom-functionalized graphene, and may provide the reason for discrepancies in recent nonlocal transport experiments on graphene.

As more transistors are packed per square mm into integrated circuits, the semiconductor industry is wrestling with a transistor overheating problem. It is believed that the solution to this problem lies in spin-electronics (spintronics, for short), which, in order to store and process classical and quantum information, exploits not only the charge of the electron but also its quantized magnetic momentum, the spin. The problem of conversion between electronic charge and spin has therefore become of paramount importance and researchers have designed many experiments to study the possible mechanisms.

Spin-charge conversion has been detected in various types of materials via non-local transport measurements, a versatile and well-established experimental technique also used to probe other important phenomena such as the (quantum) Hall effect. However, some of the existing experimental measures in two-dimensional materials like graphene functionalized with adsorbates cannot be explained by the existing transport theories. The latter typically account for only one type of spin-charge conversion, i.e. the spin Hall effect. However, in graphene decorated with adsorbates and possibly other types of two-dimensional materials, a different type of spin-charge conversion mechanism, namely the current-induced spin polarization, occurs and coexists with spin-Hall effect.

In this highlighted work, we formulated a transport theory that accounts for both types of spin-charge conversion mechanisms and uncovers two anomalous features that can help to identify which one dominates in a particular device. We observed that: i) the nonlocal resistance of a Hall bar device (see Figure 1) can take negative values (in the absence of a magnetic field) when direct magnetoelectric coupling (DMC, a form of extrinsic current-induce spin polarization) dominates the spin Hall effect (see Figure 2). ii) The nonlocal resistance under an in-plane magnetic field (the so-called "Hanle effect") can take an asymmetric shape with the reversal of the field direction (see Figure 3). Both anomalous features are caused by a direct magnetoelectric coupling which exists in disordered materials with broken inversion symmetry but was not accounted for in previous treatments. The direct magneto-electric coupling was uncovered by the present authors in an earlier work [Phys. Rev. B 94, 085414 (2016)] and it is caused by scattering with impurities that violate local inversion symmetry, i.e. Rashba spin-orbit coupling.

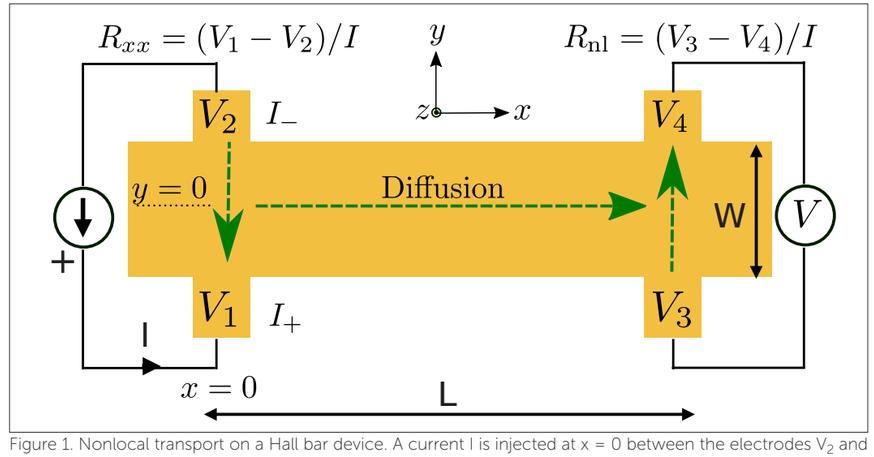


Figure 1. Nonlocal transport on a Hall bar device. A current I is injected at x = 0 between the electrodes V_2 and V_1. This gives rise to both a local resistance R_{xx} and a nonlocal resistance R_{nl}. The latter is enhanced by a process involving (i) a spin-charge conversion (current-induced spin polarization and/or spin Hall effect) at x = 0, (ii) diffusion from x = 0 to x = L, and (iii) the inverse spin-charge conversion at x = L. The green-dotted line indicates the direction of electron flow.

In certain types of two-dimensional materials, the spin Hall effect can coexist with current-induced spin polarization. We have formulated a drift-diffusion theory that accounts for both of these spin-charge conversion mechanisms and solved it on a nonlocal geometry

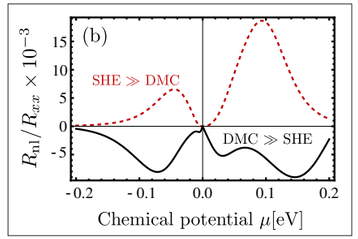


Figure 2. Nonlocal resistance R_{nl} versus the chemical potential μ of adatoms decorated graphene in the absence of a magnetic field, showing that $R_{nl} > 0$ when the spin Hall effect (SHE) dominates over directo-magnetoelectric coupling (DMC) effects, whereas $R_{nl} < 0$ when DMC dominates.

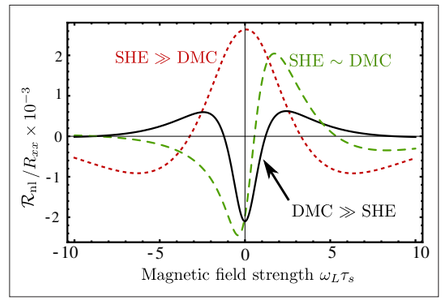


Figure 3. The Hanle precession effect (R_{nl} versus magnetic field) in the presence of direct-magnetoelectric coupling, a form of current-induced spin-polarization, and the spin Hall effect. The Hanle precession curve becomes asymmetrical when both contributions are of the same order.

DIPC HIGHLIGHT 2017

Transition-metal π-ligation of a tetrahalodiborane

H. Braunschweig, R.D. Dewhurst, J.O.C. Jiménez-Halla, E. Matito, and J.H. Muessig
Angewandte Chemie International Edition 57, 412-416 (2017)

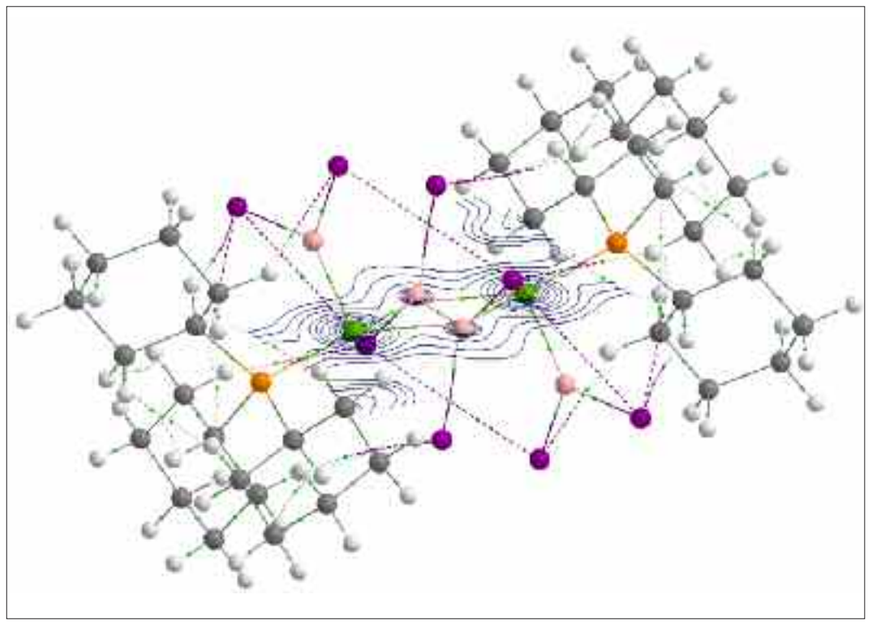
In this work we've succeeded in the synthesis of the first transition-metal complex of a diboranyl dianion, which has been computationally characterized as an olefin analogue.

Tetrahalodiboranes are enigmatic compounds formed by two boron and four halogen atoms. Despite the lability and immense reactivity potential of these structures, the relative absence of tetrahalodiboranes is due to their difficult preparation, involving gas-phase synthetic steps. As a consequence, the synthetic interest in tetrahalodiboranes ebbed after an initial spike in their use in the last century. Conversely, the filing of patents involving tetrahalodiboranes has outpaced their appearance in journal articles at a rate of two to one over the past five years. The latter is due to the versality of these intriguing compounds that, among other applications, are used for the doping of silicon with B^+ ions for semiconductor device fabrication.

Recently, the first transition-metal complex of a diboranyl dianion has been prepared and characterized by the group of Prof. Braunschweig at the University of Würzburg. The reaction of tetraiodobornae with trans-[Pt(BI_2)I(PCy_3)$_2$] gives rise to the diplatinum(II) complex [{(Cy_3P)(I_2B)Pt}$_2$(m_2:h^3:h^3-B_2I_4)], which is supported by a bridging diboranyl dianion ligand $[B_2I_4]^{2-}$.

The groups of Prof. Óscar Jimenez-Halla and Dr. Eduard Matito, an Ikerbasque Research Fellow working at the DIPC, have performed a joint computational study of these compounds using chemical bonding tools based on the topology of the electron density, electron fluctuation analysis and the intrinsic bond orbitals. The presence of ring critical points in the center of each B-Pt-B structure and the large fluctuation of the electron population among these atoms suggests the presence of two multicenter PtB_2 3c-2e bonds, similar to the two B_3 3c-2e bonds seen in Himmel's rhomboidal B_4 compound. In other words, the B_2I_4 unit can be seen as an olefin analogue.

The compound represents the first example of intact coordination of B_2X_4 (X = halide) unit of any type to a metal center. These results provide a glimpse of the potentially exciting coordination chemistry of tetrahalodiboranes, about which very little is currently known. The experimental and computational results have been published this year in *Angewandte Chemie International Edition*.



Isocountour plot of the Laplacian of the electron density around the B_2I_4 unit within the tetrahalodiborane structure.

The results provide a glimpse of the potentially exciting coordination chemistry of tetrahalodiboranes, about which very little is currently known

Imaging chemical reactions in front of a curved Pd surface: steps as active sites

S. Blomberg, J. Zetterberg, J.F. Zhou, L.R. Merte, J. Gustafson, M. Shipilin, A. Trinchero, L.A. Miccio, A. Magana, M. Ilyn, F. Schiller, J.E. Ortega, F. Bertram, H. Gronbeck and E. Lundgren
ACS Catalysis 7, 110 (2017)

It is known that atomic steps on the surface play an important role in catalytic reactions. In this work we overcome previous methodological constraints, and perform spatially resolved measurements of the CO_2 production over a cylindrical-shaped Pd catalyst to show that the light-off temperature at different parts of the crystal depends on the step orientation of the two types of steps.

Catalysts are vital for a wide range of applications in exhausts, in the chemical industry, and in energy production, because they reduce the energy barrier of chemical reactions. To further improve industrial catalysts it is essential to understand catalytic processes at the lowest atomic level. This represents a formidable challenge, implying the development of novel analytical techniques, such as the Planar Laser-Induced Fluorescence (PLIF), combined with smart experimental approaches, such as the curved crystal approach.

The PLIF technique is designed to image the gas phase in the proximity of a surface during a chemical reaction. As explained in Figure 1, a laser beam excites the molecule of interest, which relaxes by emitting a photon, and the fluorescence light is then detected. The process is highly selective, such that a specific molecule can be targeted. But it is also very intense and can implemented in a 2D fashion, such as to spatially resolve (50 μm) the gas phase of chemical reaction, for example, in front of a catalyzer.

In our experiments the target molecule was CO_2, the product molecule in the CO oxidation, and the surface was a curved Pd crystal, which acted as the catalyst. The latter is described in Figure 2 (top). The curved shape is intended to facilitate and rationalize the role of low-coordinated Pd step atoms during the CO oxidation reaction. In fact, low-symmetry vicinal surfaces with smoothly increasing density of steps sequentially appear as we move from the high symmetry (111) plane in the center and toward the edges of the sample. Using PLIF we have been able to spatially resolve the CO_2 production over the curved Pd crystal surface at different temperatures during the activation of the CO oxidation reaction. The set of PLIF images in Figure 2 (bottom) neatly demonstrate that the ignition temperature depends on step density and type, being lower at the steps named B type, and higher at the crystal center, which contains no steps.

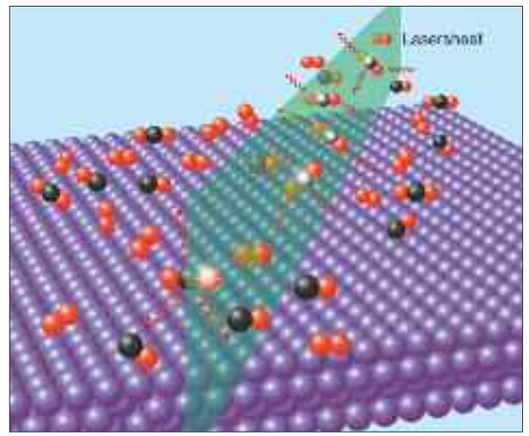


Figure 1. In Planar Laser Induced Fluorescence (PLIF) a laser beam is shaped into a laser sheet with cylindrical and spherical lenses. The laser sheet interacts with CO_2 gas molecules in the proximity of a metal surface, and the image of the CO_2 gas distribution is achieved.

By using a curved Pd crystal we were able to neatly demonstrate that the ignition temperature depends on step density and type

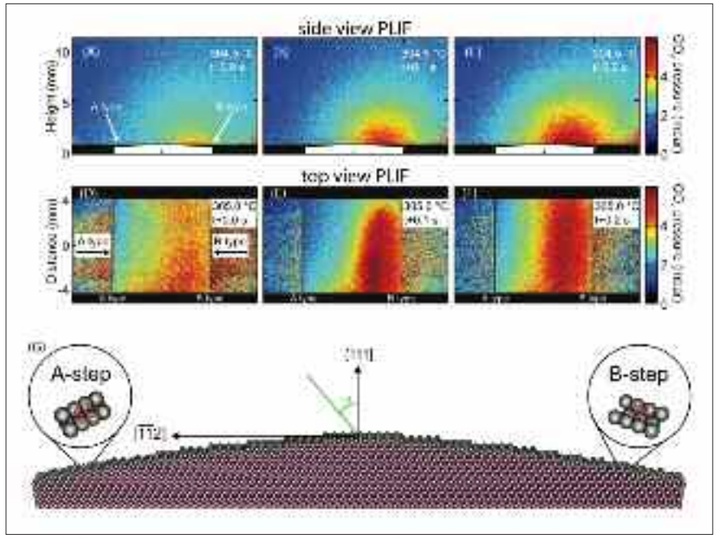


Figure 2. Bottom, schematic model of the curved Pd(111) crystal where the atomic packing of the A- and B-type steps are illustrated. Top, PLIF images (side view and top view of the curved Pd crystal) of the light-off of the CO oxidation reaction at the B-type step side at 289.5 °C, and the A- type side at 289.7 °C.

Submolecular imaging resolution using inelastic electron tunnelling spectroscopy at 5 K

B. de la Torre, M. Svec, G. Foti, O. Krejci, P. Hapala, A. Garcia-Lekue, T. Frederiksen, R. Zboril, A. Arnau, H. Vazquez, and P. Jelinek

Phys. Rev. Lett. 119, 166001 (2017)

Scanning tunneling microscopy (STM), atomic force microscopy (AFM), and inelastic electron tunneling spectroscopy (IETS) are three established techniques to image organic molecules on surfaces. Here, the three techniques are studied simultaneously by measurements using a CO-terminated tip at 5 K. The high-resolution contrast observed simultaneously in all channels unambiguously demonstrates the common imaging mechanism in STM/AFM/IETS, related to lateral bending of the CO-functionalized tip. Theoretical modeling reveals that the origin of submolecular contrast in the IETS channel consists of both a renormalization of the vibrational frequency and of a variation in the amplitude of the IETS signal.

The development of high-resolution STM, AFM, and IETS imaging with functionalized tips has allowed us to reach unprecedented spatial resolution of organic molecules on surfaces. Using these techniques, the chemical structure of molecules can now be routinely determined directly from experimental images, as well as the information about, e.g., bond order, intermediates, and products of on-surface chemical reactions. The main problem of IETS is that the high-resolution contrast was so far only demonstrated at sub-Kelvin temperatures. This temperature requirement poses severe limitations for its wider application.

In this work, an international team of researchers from DIPC and Czech institutions demonstrates for the first time that high-resolution IETS is feasible at 5 K in standard laboratory conditions and experimentally confirm the common imaging mechanism for all three imaging techniques (Figure 1).

The researchers made simultaneous AFM/STM/IETS measurements of an iron(II) phtalocyanine (FePc) molecule adsorbed on Au(111) acquired with a CO-terminated tip at 5 K. Their results demonstrate that the high-resolution IETS imaging is feasible at that temperature with a spatial resolution superior to STM and comparable to AFM. Moreover, the high-resolution contrast observed in all channels simultaneously demonstrates unambiguously the common imaging mechanism related to the lateral bending of the CO-functionalized tip. Further, the IETS spectroscopy reveals that the submolecular contrast at 5 K consists of both the renormalization of the vibrational frequency and the variation of the amplitude of the IETS signal. The team confirmed this discovery using first principles simulations, extending the probe-particle model to include these two main ingredients necessary to reproduce the high-resolution IETS contrast.

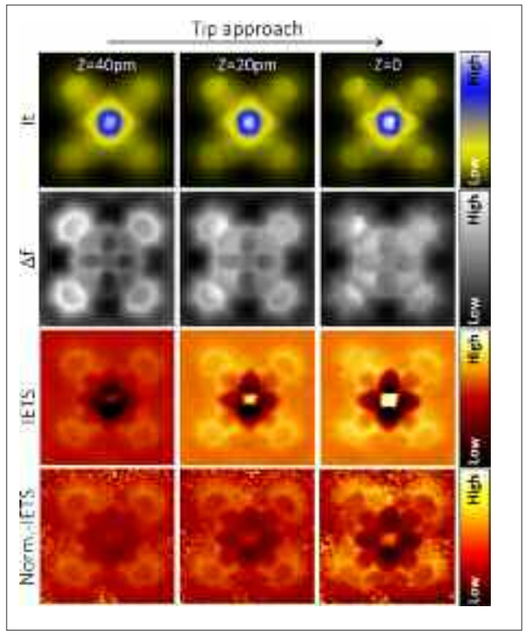


Figure 1. Simultaneous STM, AFM, and IETS constant-height images of FePc/Au(111) with a CO-functionalized tip. The tunnel current (It), the frequency shift Δf of the cantilever, IETS signal [defined here as d^2I/dV^2], and normalized IETS [$(d^2I/dV^2)/(dI/dV)$] are acquired at three different tip heights over an area of 1.6 x 1.6 nm2 with a bias voltage of 3 mV. Both Δf and IETS images show the sharp edges related with the geometric structure of the FePc molecule.

Our results demonstrate that the high-resolution IETS imaging is feasible at 5 K with a spatial resolution superior to STM and comparable to AFM

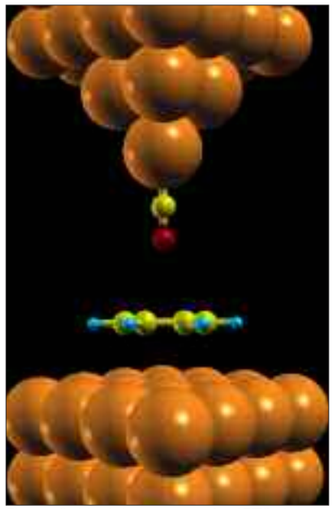


Figure 2. Model geometry for IETS simulations of a CO-terminated STM tip located over a simple organic molecule.

Band gap formation and Anderson localization in disordered photonic materials with structural correlations

L. Froufe-Pérez, M. Engel, J.J. Sáenz and F. Scheffold
Proceedings of the National Academy of Sciences of the United States of America (PNAS),
201705130 (2017)

Disordered dielectric materials with structural correlations show unconventional optical behavior: They can be transparent to long-wavelength radiation, while at the same time have isotropic band gaps in another frequency range. This phenomenon raises fundamental questions concerning photon transport through disordered media. Here, we investigate band gaps, and we report Anderson localization in 2D disordered dielectric structures using numerical simulations of the density of states and optical transport statistics.

Non-metallic solids and liquids can differ considerably one from the other from an optical point of view. An important role in this is played by the material's structure. One can find clear and transparent materials, but also opaque white or iridescently reflective ones as in the case of opals. Moreover, because of a change in structure, the same material can first be transparent and then white, as can easily be observed when frying an egg. In extreme cases, it is possible, within a particular color spectrum, to produce a perfectly reflective material.

Hyperuniform disordered, all-dielectric, structures are a new class of photonic materials which, depending on the light wavelength (color), can be perfectly transparent (like glass), they can become white (like a cloud, milk or a fright egg) and, for certain colors, behave as perfectly reflective materials (having a perfect full band gap like crystals). Uniformly disordered (amorphous) materials were first postulated in 2009 by a group of researchers at Princeton University (USA) and their unusual properties raised fundamental questions concerning the multiple scattering of light and the actual nature of Anderson localization of photons in these materials.

Now, researchers at the Universities of Fribourg (Switzerland) and Erlangen (Germany), in collaboration with J.J. Sáenz, Ikerbasque Professor at DIPC, have been successful in deciphering and systematically classifying the complete optical characteristics of so-called hyperuniform materials, as recently reported in the prestigious American journal PNAS. Using computer simulations they discover that, depending on the strength of the local ordering and wavelength of the light, entirely different optical characteristics can manifest themselves: from transparent to white or completely reflective. These findings form a basis for the design and development of modern amorphous photonic materials based on the concept of hyperuniformity.

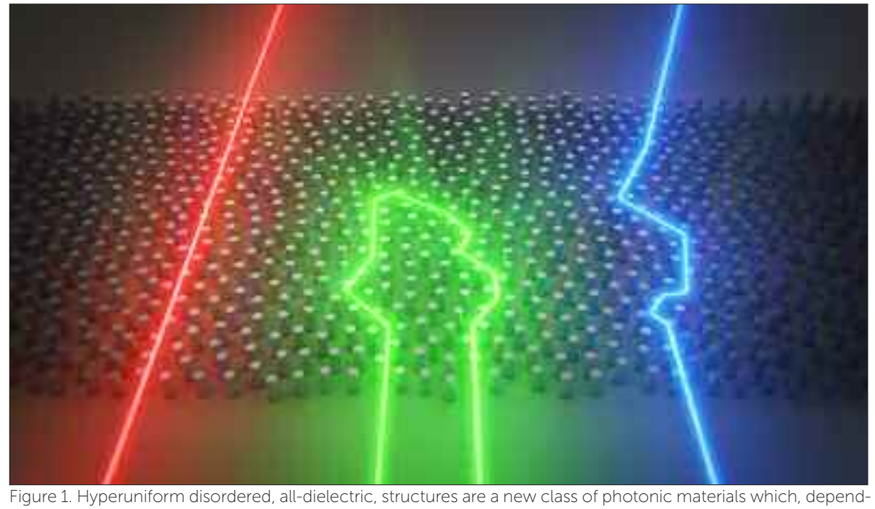


Figure 1. Hyperuniform disordered, all-dielectric, structures are a new class of photonic materials which, depending on the light wavelength (color), can be perfectly transparent (like glass), they can become white (like a cloud, milk or a fried egg) and, for certain colors, behave as perfectly reflective materials (having a perfect full band gap like crystals).

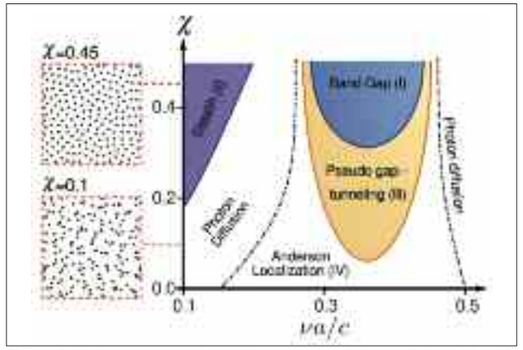


Figure 2. Light transport phase diagram were it is possible to identify all relevant regimes in a 2D system composed of silicon rods: transparency, photon diffusion, classical Anderson localization, band gap, and a pseudogap tunneling regime.

Hyperuniform disordered, all-dielectric, structures are a new class of photonic materials which, depending on the light wavelength, can be perfectly transparent, become white, and, for certain colors, behave as perfectly reflective materials

Magnetically-driven colossal supercurrent enhancement in InAs nanowire Josephson junctions

J. Tiira, E. Strambini, M. Amado, S. Roddaro, P. San-Jose, R. Aguado, F.S. Bergeret,
D. Ercolani, L. Sorba and F. Giazotto
Nature Communications 8, 14984 (2017)

In the present work we report a colossal enhancement of the critical supercurrent induced by an external magnetic field applied perpendicular to the substrate in mesoscopic Josephson junctions formed by InAs nanowires and Al superconducting leads. This striking and anomalous supercurrent enhancement cannot be described by any known conventional phenomenon of Josephson junctions. We consider these results in the context of topological superconductivity, and show that the observed critical supercurrent enhancement is compatible with a magnetic field-induced topological transition.

The coupling between a BCS superconductor (S), like Al or Nb, and a semiconducting nanowire (NW) with a strong spin-orbit coupling (SOC), like InAs or InSb may lead to unconventional p-wave superconducting correlations. Such a system may undergo a topological transition and become an artificial topological superconductor (TS) that hosts Majorana-like edge states (MS).

Majorana sates have been intensively studied in the past decades, mainly because their applicability in the development of topological quantum computation. Most of the experimental efforts to demonstrate the existence of these states have been focused on normal metal-superconductor junctions realized with strong SOC NWs with the aim to detect signatures of Majorana bound states (MBSs) in the dependence of the zero-bias conductance on an external applied magnetic field.

In the present work, which is a collaboration between the groups of Francesco Giazotto (CNR, Pisa), Ramón Aguado (CSIC, Madrid) and Sebastián Bergeret (DIPC/CFM, Donostia), we investigated the Josephson effect in a Al/InAs-NW/Al hybrid junction (see Figure 1) The Josephson effect is a fundamental quantum phenomenon where a dissipationless current (supercurrent) can flow through the junction between the two superconducting electrodes. The amplitude of this current depends on the macroscopic phase difference between S electrodes and,in clean systems it is associated to the bound states formed within the NW. The maximum supercurrent that can flow through the junction is denoted as the Josephson critical current (I_c). The latter depends on the applied magnetic field.

Measurement of I_c may provide important information about the ground state of the junction, in particular is expected to increase strongly when the topology of the junction enables the emergence of Majorana bound states.

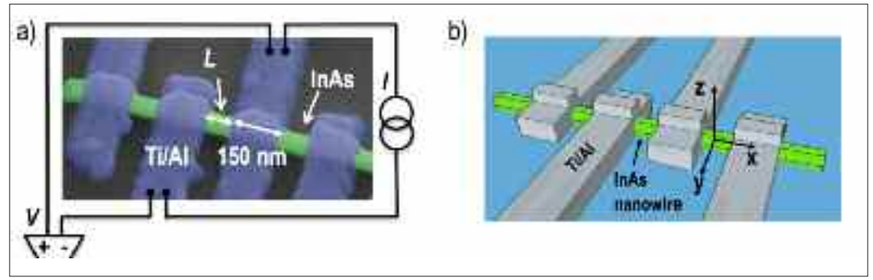


Figure 1. Sample layout: (a) Scanning electron micrograph of a typical n-InAs nanowire-based Josephson junction and sketch of the four-wire measurement setup. (b) Side view of the junction.

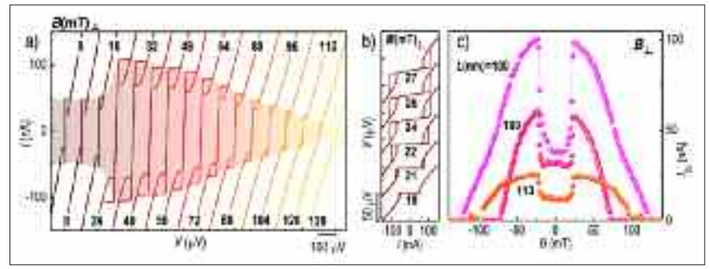


Figure 2. Enhancement of the critical current at finite out-of-plane magnetic field:
(a) Current–voltage (IV) characteristics of a Josephson junction measured for different values of the out-of plane magnetic field.
(b) Blow-up of selected IV showing the dissipative behaviour of the weak link after the transition to the enhanced I_c state.
(c) Comparison of the Ic versus B behaviour for three junctions of different length L at 15 mK.

The colossal supercurrent enhancement observed in a seminconducting Josephson junction can be explained by assuming a topological transition

Our experiment shows a striking and novel change of the amplitude of I_c when an external magnetic field is applied perpendicular to the substrate plane. As shown in Figure 2, the critical current I_c remains almost constant up to a field of 15 mT, then quickly doubles its amplitude at a switching field B_c=23mT, and I_c finally decays at larger magnetic fields. The colossal enhancement of I_c (which exceeds 100%) occurs at the same magnetic field for all the measured junctions (Figure 2c). This suggests that the origin of the effect is intrinsic to the materials combination. And is qualitatively explained by a topological transition.

Breaking bonds, forming nanographene diradicals with pressure

M. Desroches, P. Mayorga Burrezo, J. Boismenu-Lavoie, M. Peña Alvarez, C. Gómez Garcia, J.M. Matxain, D. Casanova, J.F. Morin, and J. Casado
Angewandte Chemie International Edition 56, 16212-16217 (2017)

The present study demonstrates and rationalizes how a newly synthetized anthanthrone-based polycyclic scaffold possessing peripheral crowded quinodimethanes adopt a closed-shell butterfly-shaped structure in the ground state that can easily planarize through a low energy barrier biradicaloid transition state to a low-lying diradical state. Conversion is primarily driven by the release of strain associated with steric hindrance.

Quinodimethane nanographenes with closed-shell structure experience a concave to a convex inversion through a diradical intermediate that is kinetically trapped and has a low energy lying triplet. The study reports the preparation and characterization of a new "nanographene" based on the low-cost commercially available 4,10-dibromoanthanthrene building block. While the anthanthrone core can be viewed as a fusion of two anthracene moieties with lateral functionalization, its chemical and physical properties stand in sharp contrast with the parent anthracene subunit, exhibiting remarkable stability because of its extended delocalization. We hypothesized that the general target structure shown in Figure 1 would possess an accessible diradical state upon core planarization, as this would result in the release of steric strain along with the formation of two perpendicular π-systems and overall gaining of aromatic stability. Interestingly, this system would provide a rare example of a closed-shell to diradical transition fueled by strain release.

A relatively small energy barrier for the quinoidal to diradical conversion is found that can be overcome at room temperature through fluxional inversion giving rise to a local metastable full planar structure with a net singlet diradical character and a triplet state (Figure 2). This diradical state displays most of the spin densities at the exo-acene carbon atoms. As no new Clar sextet was formed during this transformation (2 sextets in both the closed-shell and open-shell forms), the driving force for this transformation is likely attributed to the release of strain induced by the steric hindrance at the peri position of the anthanthrone.

In summary, under application of mild mechanical stress, the molecule undergoes planarization, forming a kinetically trapped diradical, which has been characterized by Raman and EPR spectroscopies in combination with quantum chemical calculations. While this rare example of π bond breaking by mechanochemistry opens the way to the generation of diradicaloid species with accessible high spin states from robust quinoidal structure, current work is focused on stabilizing the diradical state through the design of novel functionalized anthanthrone-based polycyclic aromatics.

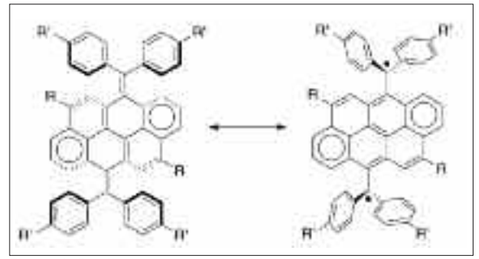


Figure 1. Studied compounds with closed-shell quinoidal and diradical canonical forms.

Under application of mild mechanical stress, the molecule undergoes planarization, forming a kinetically trapped diradical

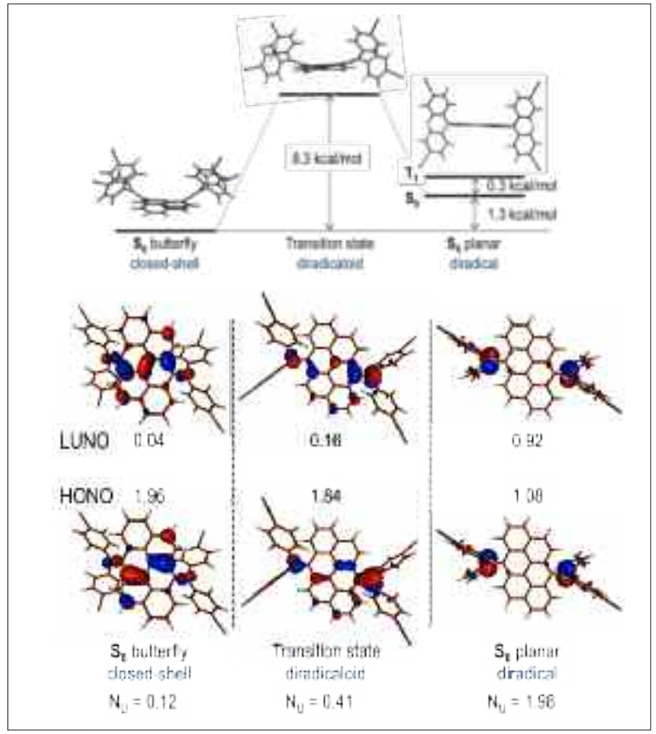


Figure 2. Top) Structures along the diradical/planar reaction path with relative Gibbs free energies and vertical singlet-triplet gaps for the planar structure. Bottom) Highest occupied natural orbital (HONO) and lowest unoccupied natural orbital (LUNO), their electron occupancies and the number of unpaired electrons (N_U) for the butterfly, TS and planar structures.

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Book Chapter

1 Designing Image Analysis Pipelines in Light Microscopy: A Rational Approach

I. Arganda-Carreras and P. Andrey

Light Microscopy: Methods and Protocols. Eds. Y. Markaki, H. Harz, Methods in Molecular Biology, Vol. 1563, pp. 185-207, Springer (2017).

DIPC COMMUNITY

Pictured here is part of the DIPC Community
at the headquarters in Donostia / San Sebastián.

DIPC HEADQUARTERS
DONOSTIA / SAN SEBASTIÁN

Researchers

Fellows Gipuzkoa

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

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

Senior Position

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).

Postdoctoral Positions

Dr. Miren Iosune Arrastia Basalo
01/08/2013–Present
Multiple spin state reactivity in Fe-containing complexes and enzymes.

Dr. Federica Lo Verso
01/02/2014–31/01/2017
Structure and dynamics of complex materials based on polymers.

Dr. Romain Dupuis
10/12/2014–09/12/2017
Computational studies on calcium silicate hydrates.

Dr. Joseba Alberdi Rodriguez
01/07/2015–Present
Morfokinetics: development of computational techniques for the analysis of CVD growth of new 2D materials.

Dr. Marta Pelc
01/12/2015–Present
Topological defects on carbon like nanostructures.

Dr. Omjyoti Dutta
01/01/2016–31/12/2017
Quantum matter and quantum simulations at the interface of optics and solid state physics.

Dr. Daniel Martinez Tong
11/01/2016–Present
Local dielectric spectroscopy by AFM. Application to polymer based materials.

Dr. Mathias Ljungberg
01/04/2016–31/03/2017
Model calculations of solid organic/inorganic interface.

Dr. Carlos Garcia Fernandez
20/04/2016–Present
Development of transport methods based on Wannier function.

Dr. Mario Zapata Herrera
01/07/2016–Present
Quantum and classical approaches to the optical response of metallic nanostructures.

Dr. Pawel Nita
01/08/2016–31/07/2017
Functional materials synthesized by surface-supported chemistry under vacuum.

Dr. Jon Iñaki Mujika
16/08/2016–Present
Molecular dynamics of membrane structure.

Dr. Aleksander Victorovich Terentjev
01/09/2016–Present
Time dependent density functional theory beyond the local density approximation.

Dr. Jorge Budagosky Marcilla
01/10/2016–Present
Computational solid state spectroscopy.

Dr. Victor Escobedo Bermudez
01/10/2016–27/10/2017
Literature and science.

Dr. Nuno De Sousa
08/11/2016–07/06/2017
Light scattering, emission rates and optical forces in colloidal suspensions.

Dr. Maxim Ilin
16/12/2016–Present
Upgrade of MOKE setup to add up the capability for as-susceptibility measurements.

Dr. Luca Bergamini
01/01–31/12/2017
Optical response of nano-antennas and novel materials.

Dr. Beatriz Robles
01/01/2017–Present
Dynamic properties of concentrated solutions of single chain nanoparticles.

Dr. Yao Zhang
01/01–31/12/2017
Atomistic description of surface enhanced raman scpectroscopy.

Dr. Rafael Grande Aztatzi
13/03/2017–Present
Molecular dynamics of Al protein interactions.

Dr. Deung Jang Choi
01/05/2017–Present
Magnetic states on superconducting surfaces.

Dr. Luciano Colazzo
26/06/2017–Present
Functional materials synthesized by surface-supported chemistry under vacuum.

Dr. Susana Velasco
10/07–07/09/2017
Developing catalytic and photocatalytic assays under biologically relevant conditions.

Dr. Jens Herwig Brede
01/09–31/12/2017
Physical chemical reactions at surfaces: physico-chemical aspects.

Dr. Pedro Brandimarte Mendonca
01/10/2017–Present
Electronic structure and quantum transport in graphene based nanostructures and networks.

Dr. Alejandro Rivero Santamaría
09/10/2017–Present
Dynamics of elementary reactive processes at surfaces.

Dr. Jhon Wilfer Gonzalez Salazar
01/11/2017–31/01/2018
Electronic and magnetic properties of 2D materials and small clusters.

Dr. Xavier Monnier
15/11/2017–Present
Ultra dense/low energy state glasses by agin nanostructured polymers.

Dr. Paula Malo de Molina Hernandez
15/12/2017–Present
All polymer nano composites: effect of soft nano objects on polymer structure and dynamics.

PhD Students

Anton Xose Brion Rios
06/02/2013–Present
Theoretical study on the molecular adsorption and self-organization on substrates of different nature.

Dino Novko
25/09/2013–10/04/2017
Non-adiabatic effects in the interaction of metal surfaces with atoms and small molecules.

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.

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

Jon Lafuente Bartolomé
01/01/2016–12/03/2017
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.

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

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

Olatz Uranga Barandiaran
15/11/2016–22/01/2017
Theoretical and computational studies of excited states in molecules and aggregates.

Irene Casademont
01/01/2017–22/01/2017
Computational studies of molecular photosensitizers.

María Eugenia Sandoval Salinas
11/01/2017–28/02/2017
Photopysical processes in complex systems.

Peio Garcia Goiricelaya
01/02/2017–Present
Spinorial structure of the electron-phonon interaction in surfaces with stron relativistic corrections.

Donaldi Mancelli
03/02/2017–Present
Experimental and theoretical analysis of simple compounds under shock-wave compression

José Reina Galvez
01/03/2017–15/04/2017
DFT calculations of the electronic structure of Co and Fe atoms on MgO.
Calculations of multiplets, with SOC. Derivation of an "effective spin Hamiltonian".

María Blanco De Paz
27/03/2017–Present
Spin orbit interactions in photonic systems.

Juan Gurruchaga Pereda
03/04/2017–Present
Photocatalytic upconverting nanomaterials for metal based photochemotherapy.

Moritz Müller
09/06/2017–Present
Lifetimes of HOMO and LUMO states of organic molecules relevant for organic photovoltaics on different substrates.

Xianpeng Zhang
11/07/2017–Present
Spin and charge transport in low dimensional systems and hybrid structures.

Alvaro Nodar Villa
01/09/2017–Present
Quantum approaches to the interaction of molecules and plasmonic excitations in nanophotonics.

Mikel Olano Aramburu
01/09/2017–Present
Quantum information processing with electrons and phonons in semiconductors.

Xabier Telleria Allika
04/09/2017–Present
Statically screened potentials, Hookean systems and quantum dots.

Sofia Sanz Wuhl
07/09/2017–Present
Theory of quantum transport in graphene based nanostructure networks.

Antton Babaze
01/10/2017–Present
Quantum approaches to the interaction of molecules and plasmonic excitations in nanophotonics.

Raúl Guerrero Avilés
27/10/2017–Present
Adsorbing atoms and molecules on van der Waals heterostructures.

Mohammed Sabri Gamal Mohammed
01/11/2017–Present
Functional materials synthesized by surface-supported chemistry under vacuum.

Haritz Garai Marin
15/11/2017–Present
Relaxation of electronic states of magnetic add-atoms at surfaces considering numerical renormalization group (NRG).

Iñigo Robredo Magro
16/11/2017–Present
Looking for new fermions in conventional crystals.

Mikel Arruabarrena
01/12/2017–Present
TDDFT approach for the direct calculation of exciton binding energies.

Internships

Igor Cortés Cejudo
UPV/EHU
03/10/2016–31/01/2017
Virtual machines cluster Installation.

Miriam Rico Medina
UPV/EHU
03/10/2016–31/01/2017
Energy saving system for the computer clusters.

Aritz Olea Zubikarai
UPV/EHU
01/02–31/03/2017
Security appliance installation for the I2basque network.

Ivan Escalante Crespan
UPV/EHU
01/02–31/05/2017
Monitoring HPC Clusters.

Iker Moya González
UPV/EHU
01/02–31/05/2017
Monitoring micro-computing equipment.

Edorta Beitia Lobato
UPV/EHU
15/05–28/07/2017
Installation and configuration of a mail server for sensors & queue systems.

Silvia García García
UPV/EHU
15/05–14/07/2017
Installation and configuration of advertising displays.

Edgar Orosa Paz
UPV/EHU
01/06–31/07/2017
Improvement of the utilization of DIPC computational resources.

Josu Salinas Colina
UPV/EHU
01/06–31/07/2017
Development of open-source software for the unsupervised segmentation of bio-medical images.

Maialen Galdeano Fraile
UPV/EHU
08/06–07/08/2017
DFT calculations of charged graphene flakes.

Unai Muniain Caballero
UPV/EHU
12/06–11/08/2017
Quantum effects in plasmonic gratings.

Martín Callejo Arroyo
UPV/EHU
15/06–14/08/2017
Quantum transport in graphene-based nanodevices.

Jon Lasa Alonso
Universidad de Salamanca
15/06–15/08/2017
Sensing capabilities of nanophotonic devices.

Joseba Goikoetxea Perez
Universidad Autónoma de Madrid
03/07–31/08/2017
Quantum interference effects due to spin fields in mesoscopic rings.

Jaime Saez Mollejo
Universidad Autónoma de Madrid
03/07–03/09/2017
Simulation of electronic properties in graphene nanostructures.

Silvia Escayola Gordils
Universidad de Gerona
15/07–15/09/2017
Short-range DFT correlation within the RAS-SF method.

Martí Gimferrer Andrés
Universidad de Gerona
15/07–15/09/2017
Electron correlation in intracules functions of the pair density.

Adriana Faraone
University of Bologna, Italy
26/07–26/09/2017
Development of photoactivatable nanomaterias for chemotherapy.

Daniel Ruiz Fulgencio
UPV/EHU
01/08–30/09/2017
Isolation of cyclic oligomers of poly(ethylene oxide) from blends by selective intercalation into graphite oxide.

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 photoelectron 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.

Prof. Luca Salassa
Development of photoactivatable anticancer metal complexes and nanomaterials. Experimental and computational inorganic photochemistry.

Prof. Denis Vyalikh
Photoemission measurements of magnetic surface states.

Ikerbasque Research Fellows

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

Dr. Rubén Esteban Llorente
01/01/2017–Present
Tema de investigación: Quantum plasmonics.

Ikerbasque Research Associates

Dr. Marek Grzelczak
01/09/2017–Present
Synthesis and self-assembly of plasmonic nanoparticles for photochemical applications.

Dr. Arantzazu Garcia Lekue
01/11/2017–Present
Modeling electron transport at the nanoscale. Theoretical investigation of electron processes at nanostructured surface.

Dr. Paola Ferrario
01/12/2017–Present
Neutrino physics.

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. Sara Barja UPV/EHU
Dr. Aitor Bergara UPV/EHU
Dr. Sebastian Bergeret CSIC
Dr. Maria Blanco UPV/EHU
Dr. Igor Campillo Euskampus
Dr. Daniele Cangialosi CSIC
Dr. David Casanova UPV/EHU
Dr. Miguel Ángel Cazalilla CSIC
Dr. Silvina Cerveny CSIC
Prof. Eugene Chulkov UPV/EHU
Dr. Martina Corso CSIC
Prof. Fernando Cossio UPV/EHU
Dr. David De Sancho UPV/EHU
Dr. Asier Eiguren UPV/EHU
Dr. Ion Errea UPV/EHU
Prof. Joaquín Fernández UPV/EHU
Dr. Idoia García de Gurtubay UPV/EHU
Prof. Francisco José García Vidal UAM
Dr. Miguel Angel Gosalvez UPV/EHU
Dr. Iñaki Juaristi UPV/EHU
Dr. Stefan Kurth 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
Dr. Miguel Moreno Ugeda UPV/EHU
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
Dr. Ilya Tokatly UPV/EHU
Prof. Jesus M. Ugalde UPV/EHU
Prof. Lucia Vitali UPV/EHU
Dr. Nerea Zabala UPV/EHU

Visiting Researchers

Long visits

Yuri Hasegawa
University of Tsukuba, Japan
22/08/2016–15/02/2017
Self-assembled and covalently-coupled molecular networks on metallic surfaces.

Prof. Talat Shahnaz Rahman
University of Central Florida, USA
01/12/2016–01/02/2017
Surface coordination chemistry and development of many-body theories beyond DFT.

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

Prof. Bogdan Andrei Bernevig
Princeton University, New Jersey, USA
15/01–05/03/2017
Topological matter: classification and design.

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

Prof. Vito Despoja
University of Zagreb, Croatia
01/02–01/03/2017
Optical properties of quasi-two-dimensional crystals.

Grabiele Dalla Torre
Universita degli Studi di Milano, Italy
01/09/2015–30/04/2017
Theoretical approach to aluminum biochemistry: developments of new chelation therapies

Dr. Roman Kuzian
National Academy of Sciences of Ukraine,
Kiev, Ukraine
01/02–30/04/2017
Photoemission from strongly correlated systems.

Prof. Wolfgang Schattke
Institut für Theoretische Physik,
Christian-Albrechts-Universität zu Kiel, Germany
01/02–30/04/2017
Molecular machines on surfaces:
Benzene and derivates.

Prof. Marijan Sunjic
University of Zagreb, Croatia
01/02–28/02/2017
Dynamical response and surface excitations in thin films.

Nick Gerrits
Leiden Institute of Chemistry, Netherlands
02/02–12/05/2017
Atoms in jellium beyond the local density approximation. Implications for electronic friction.

Prof. Joseph Richard Manson
Clemson University, South Carolina, USA
06/02–15/03/2017
Electron-phonon interaction at surfaces.

Prof. Gabriel Cwilich
Yeshiva University, New York, USA
13/02–31/07/2017
Work in several projects onpropagation in random media, quantum optics and collaborate with the program Mestizajes

Azar Ostovan
Shahid Chamran University of Ahvaz, Iran
18/02–10/08/2017
The ab-initio simulations of electron transport in nanoscale devices.

Prof. Peter Saalfrank
Institut für Chemie, Universität Postdam,
Postdam-Golm, Germany
01/03–31/03/2017
Theory of electronic friction at surfaces.

Dr. Bruce Milne
Universidade de Coimbra, Coimbre, Portugal
12/03–26/08/2017
Predicting properties of biogenic materials with machine learning.

Prof. Andrey Borissov
ISMO, Université Paris-Sud, Orsay Cedex, France
01/04–31/05/2017
Quantum Plasmonics.

Prof. Gernot Frenking
Philipps-Universität Marburg, Germany
01/04–31/07/2017
Advances in chemical bonding theory.

Prof. Bogdan Andrei Bernevig
Princeton University, New Jersey, USA
24/04–05/06/2017
Topological matter: classification and design.

Malin Kück
Humboldt-University Berlin, Germany
01/05–31/07/2017
Introduction to scattering and optical forces at the nanoscale.

Prof. Vladimiro Mújica Hernandez
Arizona State University, USA and Yachay Tech, Ecuador
01/05–31/05/2017
Effective spin-orbit interaction in chiral molecules. Field-induced chirality transfer. Chiral-induced asymmetry in CP MAS NMR.

Manon Gouspy
Université Paris Sud, Orsay, France
08/05–08/08/2017
Preparation and structural characterization of a nanostructured surface in ultra high vacuum.

Prof. Andrey Vasenko
Moscow Institute of Electronics and Mathematics, Russia
16/05–15/08/2017
Electronic transport in topological insulators.

Prof. Bo Hellsing
Gothenburg University, Sweden
01/06–31/07/2017
Electron-phonon couling in graphene.

Dr. Tatiana Menshchikova
Tomsk State University, Russia
01/06–28/08/2017
Investigation of the electronic structure of topological insulators using first-principles calculations.

Prof. Oleg V. Prezhdo
University of Southern California, USA
01/06–31/08/2017
Modeling of excitation dynamics in nanoscale materials using time-domain density functional theory and advanced techniques

Dr. Igor Rusinov
Tomsk State University, Russia
01/06–28/08/2017
Investigation of the Weyl semimetal, topologically non trivial systems using first-principles and model calculations.

Prof. Juan Faustino Aguilera Granja
UASLP, Universidad Autónoma San Luis Potosí, México
03/06–04/08/2017
Electronic and structural properties of two dimensional systems and cobaltocenos.

Prof. Talat Shahnaz Rahman
University of Central Florida, Orlando, Florida, USA
03/06–01/07/2017
Theoretical and computational investigation of chemical reactivity, electrical transport, and multiple excitations, and ultrafast processes in functional 2D materials.

Prof. Maria Angeles Hernandez Vozmediano
Instituto de Ciencia de Materiales (CSIC), Madrid, Spain
08/06–08/07/2017
Topological matter.

Prof. Alfredo Correa
Lawrence Livermore National Laboratory, California, USA
12/06–15/07/2017
Electron dynamics.

Prof. Miguel Angel Cazalilla Gutierrez
National Tsing Hua University, Taiwan
15/06–15/09/2017
Spintronics at interfaces and 2D materials.

Wen Wan
Xiamen University, Fujian, China
15/06–15/09/2017
Growth of 2D materials by MBE and electronic characterization by STM/STS.

Dr. Maxim Kharitonov
Würzburg University, Germany
16/06–31/07/2017
Topological superconductivity.

Prof. Pavel Jelínek
Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic
19/06–30/07/2017
Molecular nanostructures on surfaces.

Prof. Arthur Ernst
Institut für Theoretische Physik,
Johannes Kepler Universität, Linz, Austria
01/07–31/07/2017
Magnetism in topological insulators.

Prof. Francisco José Garcia Vidal
Universidad Autónoma de Madrid, Spain
01/07–31/08/2017
Quantum plasmonics.

Prof. Francisco Guinea López
Imdea Nanociencia, Madrid, Spain
01/07–31/07/2017
Condensed matter theory.

Prof. Nikolay Kabachnik
Institute of Nuclear Physics,
Moscow State University, Russia
01/07–30/09/2017
Study of Auger processes in gases and at solid surfaces within an attosecond streaking scheme.

Dr. Ziya Aliyev
Azerbaijan State Oil and Industry University, Baku, Azerbaijan
06/07–30/09/2017
Material physics of topological insulators.

Prof. Luis Martin Moreno
Instituto de Física de Materiales de Aragón, Universidad de Zaragoza, Zaragoza, Spain
07/07–06/08/2017
Theory on nanophotonics.

Dr. Sergey Eremeev
Institute of Strength Physics and Materials Science, Tomsk. Russia
08/07–07/09/2017
Electronic structure of topological insulators.

Prof. Jorge Kohanoff
Queen's University Belfast, School of Mathematics and Physics, Belfast, UK
08/07–18/08/2017
Dynamical simulation of irradiation processes.

Carmelo Nim
Università degli Studi di Pisa, Italy
10/07–10/08/2017
Analysis of density functionals from the study of intracule functions.

Prof. Bogdan Andrei Bernevig
Princeton University, New Jersey, USA
01/08–31/08/2017
Topological matter: classification and design.

Prof. Vito Despoja
University of Zagreb, Croatia
01/08–30/09/2017
Plasmons in quasi two dimensional crystals.

Dr. Andrey Kuznetsov
Tomsk State University, Russia
01/08–31/08/2017
Investigation of the electronic structure of topological insulators using first-principles calculations.

Prof. Vladimir Kuznetsov
Tomsk State University, Russia
01/08–31/08/2017
Investigation of the electronic structure of topological insulators using first-principles calculations.

Prof. Vladimir Menshov
National Research Centre, Kurchatov Institute, Moscow, Russia
07/08–31/10/2017
QAHE in heterostructures topological insulator / magnetic normal insulator.

Prof. Pedro De Andrés
Instituto de Ciencia de Materiales (CSIC), Madrid, Spain
01/09–30/09/2017
Lifetime of image states in thin films.

Prof. Ceferino Lopez Fernandez
Instituto de Ciencia de Materiales (CSIC), Madrid, Spain
01/09–30/09/2017
Disorder photonics.

Dr. Rubén Miguel Ochoa de Zuazola
Hitachi Cambridge Laboratory, University of Cambridge, England
01/09/2017
Skyrmions.

Sebastian Pawel Sitkiewicz
Universidad de Valencia, Spain
01/09–30/09/2017
Development of density functions for the calculation of nonlinear optical properties.

Mohammed Sabri Gamal Mohammed
Sudan University of Science and Technology, Sudan
04/09–31/10/2017
Functional materials synthesized by surface-supported chemistry under vacuum.

Prof. Amand Lucas
University of Namur, Belgium
11/09–31/10/2017
Surface physics. Book writing

Dr. Marco Evangelisti Crespo
CSIC, Instituto de Ciencia de Materiales de Aragón, Universidad de Zaragoza, Spain
16/09–31/10/2017
Molecular magnetism.

Prof. Joseph Richard Manson
Clemson University, Clemson, South Carolina, USA
20/09–10/11/2017
Electron-phonon interaction at surfaces.

Ifeanyi John Onuorah
University of Parma, Italia
20/09–20/10/2017
Anharmonic effects for muon studies

Haritz Garai Marin
Universidad del País Vasco/Euskal Herriko Unibertsitatea, Leioa, Spain
01/10–14/11/2017
Relaxation of electronic states of magnetic add-atoms at sufaces considering numerical renormalization group (NRG).

Dr. Igor V. Silkin
Tomsk State University, Russia
16/10–15/12/2017
Topological insulators.

Dr. Jorge Luis Hita
Universidad Autónoma de Madrid, Spain
22/10–22/12/2017
Dipolar interactions between nanoparticles induced by random electromagnetic fields.

Prof. Yury Koroteev
Institute of Strength Physics and Materials Science, Siberian Branch of Russian Academy of Sciences, Russia
23/10–23/12/2017
Topological insulators.

Prof. Julio A. Alonso Martín
Universidad de Valladolid, Spain
01/11–30/11/2017
Interaction of hydrogen with metallic nanoparticles.

Prof. Alexander Protogenov
Institute of Applied Physics, Russian Academy of Sciences, Nizhnii Novgorod, Russia
01/11–30/11/2017
Landau damping of collective exitations in Dirac materials.

Prof. Luis Alberto Montero Cabrera
Universidad de La Habana, Cuba
12/11–22/12/2017
Understanding singlet fission as a photonic enhancing effect.

Dr. Chunli Huang
National Tsing Hua University, Hsinchu City, Taiwan
23/11/2017–23/01/2018
Spintronics of low-dimensional materials and interfaces.

Reece Roberts
Macquarie University, New South Wales, Australia
11/12/2017–11/01/2018
Levitation of nanodiamonds.

Short visits

Prof. Lawrence Glasser
Clarkson University, New York, USA
15/01–21/01/2017
Second order exchange energy of graphene.

Diego Romero Abujetas
Instituto de Estructura de la Materia, IEM-CSIC, Madrid, Spain
16/01–27/01/2017, 19/06–08/07/2017, 11/12–22/12/2017
Theory of light scattering in nano-structured highly refractive media.

Prof. Raffaele Resta
Università di Trieste, Trieste, Italy
02/01–21/01/2017, 05/02–18/02/2017
Geometry and topology in electronic structure.

Prof. Godfrey Gumbs
Hunter College, City University of New York, USA
06/01–27/01/2017
Electronic properties of black phosphorus in perpendicular electric and magnetic fields.

Julie Baumard
LOMA and Université de Bordeaux, France
09/01–13/01/2017
Spin, charge and heat transport in superconducting nanostructures with generic spin fields.

Dr. Jerome Cayssol
Université Bordeaux, LOMA, France
09/01–11/01/2017
Quantum transport in excitonic condensates.

Dr. Zhi Jun Wang
Princeton University, New Jersey, USA
16/01–05/02/2017
Topologically ordered phases of matter.

Prof. Alexander Khaetskii
University at Buffalo, SUNY, New York, USA
18/01–22/01/2017
Stimulated phonon emission at the nanoscale.

Dr. Oliver Gröning
EMPA, Switzerland
23/01–26/01/2017
On-surface synthesis and properties characterization of novel low-dimensional materials.

Dr. José Ignacio Latorre
Universidad de Barcelona, Spain
25/01–26/01/2017
History of physics: the Manhattan project.

Prof. Pawel Rejmak
Institute of Physics, Polish Academy of Sciences, Warsaw, Poland
01/02–15/02/2017
Computational studies on cement materials.

Dr. Sergio Monturet Caamaño
EIT Raw Materials, Bordeaux, France
02/02–04/02/2017
EIT as a financial source for collaboration among industry and research groups.

Prof. Francisco Javier Muñoz Saez
Universidad de Chile, Santiago, Chile
05/02–24/02/2017
Topological materials.

Prof. Felipe Pinheiro
Federal University of Rio de Janeiro, Brazil and Optoelectronics Research Centre, Southampton, England
05/02–08/02/2017
Natural optical activity in disordered media.

Jorge Luis Hita
Universidad Autónoma de Madrid, Spain
09/02–03/03/2017
Theoretical analysis of optical binding induced by random field fluctuations.

Dr. Barry Bradlyn
Princeton University, New Jersey, USA
11/02–19/02/2017, 10/07–08/08/2017
Topological quantum chemistry.

Quentin Schaeverbeke
Laboratoire Ondes et Matiére d'Aquitaine (LOMA) Universit de Bordeaux et CNRS, Talence, France
13/02–17/02/2017, 30/05–02/06/2017, 13/11–14/11/2017
Dynamical aspects of quantum transport in nanoelectronics.

Jennifer Cano
Princeton University, New Jersey, USA
14/02–01/03/2017
Topological materials.

Prof. Juan Luis Mañes
Facultad de Ciencia y Tecnología, Leioa, Spain
17/02–17/02/2017
Weyl fermions from crystal symmetry.

Prof. Giorgio Benedek
Universitá di Milano-Bicocca, Milano, Italy
20/02–26/02/2017, 06/10–14/10/2017
Surface phonons and phase transitions.

Prof. Jakub Zakrzewski
Uniwersytet Jagiellonski, Krakow, Poland
20/02–20/02/2017
Ultracold gases in shaken optical lattices.

Prof. Salvador Miret Artes
CSIC, Instituto de Física Fundamental, Madrid, Spain
21/02–23/02/2017, 08/10–12/10/2017
Theory of surface diffusion.

Johannes Falke
TU Dresden, Germany
26/02–03/03/2017
Interplay of crystal electric field states with spin-polarized surface states in heavy-fermion materials.

Prof. Tomasz Sowinski
Quantum Optics Group, Institute of Physics of the Polish Academy of Sciences, Warsaw, Poland
01/03–02/03/2017
Dipolar molecules in optical lattices.

María Blanco De Paz
CSIC, Instituto de Física Fundamental, Madrid, Spain
02/03–04/03/2017
Spin orbit interactions in photonic systems.

Prof. Román Orús Lacort
Johannes Gutenberg-Universität Mainz, Germany
05/03–01/04/2017
Quantum many body systems and quantum information.

Prof. Vladimir Menshov
National Research Centre, Kurchatov Institute, Moscow, Russia
07/03–05/04/2017
QAHE in heterostructures topological insulator / magnetic normal insulator.

Dr. Paula Natalia Abufager
Instituto de Física Rosario-CONICET, Argentina
12/03–08/04/2017
Electronic properties at the nanoscale.

Prof. François Lagugné-Labarthet
Western University, London, Ontario, Canada
16/03–16/03/2017
Enabling sensing technology with plasmonics.

Dr. Marco Evangelisti Crespo
CSIC, Instituto de Ciencia de Materiales de Aragón, Universidad de Zaragoza, Spain
23/03–24/03/2017
Molecular magnetism.

Sabine Auras
Universiteit Leiden, Netherlands
26/03–14/04/2017
Statistical analysis of terrace width distributions on curved crystals.

Prof. Bo Hellsing
Göteborgs Universitet, Sweden
27/03–06/04/2017
Electron-phonon couling in graphene.

Dr. Federica Giulia Lo Verso
Syddansk Universitet, Odense, Denmark
27/03–31/03/2017
Computer simulations of nanogels.

Prof. Juan Faustino Aguilera Granja
UASLP, Universidad Autónoma San Luis Potosí, México
02/04–30/04/2017, 11/12–06/01/2018
Electronic and structural properties of two dimensional systems.

Prof. Miguel Angel Martín Delgado Alcántara
Universidad Complutense de Madrid, Spain
05/04–09/04/2017
Topological codes in quantum information; topological order in spin systems.

Prof. Thomas Weitz
LMU Munich, Germany
05/04–07/04/2017
Charge transport in organic nanoscopic systems: From organic semiconductors to 2d layered materials.

Dr. Shigeki Kawai
MANA, Tsukuba, Japan
10/04–14/04/2017
X-ray photoemission from graphene nanorribbons grown by on-surface reactions.

Dr. Raúl Angulo
Centro de Estudios de Física del Cosmos de Aragón, CEFCA, Teruel, Spain
24/04–27/04/2017
Numerical simulations in cosmology.

Rishav Harsh
Université Paris-Diderot, Laboratoire Matériaux et Phénomènes Quantiques, Paris, France
26/04–05/05/2017
Donor-acceptor molecular assemblies on graphene/SiC(0001).

Dr. Miztli Yepez
Universidad Metropolitana Iztapalapa, México
29/04–08/05/2017
Theoretical work on multiple scattering of light.

Prof. Christoph Rossel
IBM Research, Zurich, Switzerland and European Physical Society
03/05–07/05/2017
From nanoscale systems to neuromorphic computing.

Prof. Yaroslav Pavlyukh
Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Germany
07/05–11/05/2017
Cumulant expansions in MBPT_LCAO.

Prof. Chris Exley
The Birchall Centre, Lennard-Jones Laboratories, Keele University, Staffordshire, UK
08/05–12/05/2017
Aluminium in biological systems.

Johannes Knörzer
MPI für Quantenoptik (MPQ), Garching, Germany
08/05–13/05/2017
Acoustic lattice for electrons.

Dr. Martin Schütz
Harvard University, Massachusetts, USA
08/05–13/05/2017
Acoustic lattice for electrons.

Dr. Benjamin Wieder
Princeton University, New Jersey, USA
08/05–26/05/2017, 12/07–31/07/2017
Basic research exploring new frontiers in quantum condensed matter physics and physical chemistry.

Prof. Thierry Martin
Centre de Physique Théorique (CPT), Université Aix-Marseille, France
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Electronic quantum optics.

Prof. Dilgam Taghiyev
Institute of Catalysis and Inorganic Chemistry, Azerbaijan National Academy of Sciences, Baku, Azerbaijan
23/05–30/05/2017
Advanced materials for spintronics and quantum computing (AMSQC).

Dr. Magdalena Marganska-Lyzniak
Universität Regensburg, Germany
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Topological invariants and boundary states in normal and superconducting carbon nanotubes.

Dr. Remi Avriller
CNRS Laboratoire Ondes et Matière d'Aquitaine (LOMA) Université de Bordeaux et CNRS, Talence, France
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Dynamical aspects of quantum transport in nano-electronics.

Tatiana Woller
VUB, Vrije Universiteit Brussel, Belgium
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Aromaticity and delocalization in expanded porphyrins.

Prof. Toru Hirahara
Tokyo Institute of Technology, Tokyo, Japan
04/06–07/06/2017
Topological insulators: magnetism and quantum anomalous hall effect.

Dr. Ian Osborne
Science Magazine
05/06/2017

Dr. Alberto Cortijo Fernandez
Instituto de Ciencia de Materiales, CSIC, Madrid, Spain
07/06–08/06/2017
Unconventional magnetotransport in Weyl semimetal.

Prof. Bernhard Urbaszek
CNRS Toulouse University, France
09/06–10/06/2017
Optical properties of 2D semiconductors in van der Waals heterostructures.

Prof. Damien Thompson
University of Limerick, Ireland
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Can nanoscale computer simulations aid the rational design of new materials?

Prof. Andrew Gellman
Carnegie Mellon University, Pennsylvania, USA
14/06–15/06/2017
Fabrication of spherical crystals.

Prof. Richard M. Martin
University of Illinois, Palo Alto, USA
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Electronic structre of solids, especially topological insulators.

Prof. Dietrich Menzel
Technische Universität München, Garching and Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany
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Ultrafast charge transfer at surfaces.

Prof. Jaroslav Fabian
University of Regensburg, Germany
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Spin-orbit and exchange proximity effects in 2d materials.

Prof. Gabriel Molina Terriza
Macquarie University, Sydney, Australia
22/06–01/07/2017
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Lorenzo Monacelli
Universitá di Rome La Sapienza, Italy
26/06–24/07/2017
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Prof. Vladimir Chaldyshev
Ioffe Physico-Technical Institute, Russian Academy of Science, St. Petersburg, Russia
01/07–12/07/2017
Plasmonic properties of metal nanoparticles in semiconducting materials.

Prof. Justin W. Wells
Norwegian University of Science and Technology (NTNU), Trondheim, Norway
03/07–07/07/2017
Electron-phonon coupling in graphene.

Dr. Andrés Anca Couce
Graz Univerity of Technoloy, Austria
06/07–08/07/2017
Biomass pyrolysis to produce biochar.

Dr. Miguel Martinez Canales
The University of Edinburgh, UK
06/07–01/08/2017
Dirac fermions in boron halide monolayers.Martensitic transformations in the alkali metals. High pressure phases in the noble metals.

Prof. Javier Garcia de Abajo
ICFO-Instituto de Ciencias Fotonicas, Castelldefels, Barcelona, Spain
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Theoretical aspects of the interaction of light with nanostructures.

Rodrigo Humberto Aguilera Del Toro
Universidad de Valladolid, Spain
09/07/2014–14/07/2017
Electronic properties of clusters.

Dr. Masaki Tezuka
Kyoto University, Japan
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Dynamics of low-dimensional strongly-correlated systems.

Shaffique Adam
Yale-NUS College, Singapore
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The role of electron-electron interactions in graphene.

Prof. Ming-Chiang Chung
National Chung-Hsing University, Taichung, Taiwan
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Dr. Massimo Rontani
Cnr-Nano, Modena, Italy
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Prof. Dmitry Usachov
Saint Petersburg State University, Russia
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Prof. Alexander Golubov
University of Twente, Netherlands
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Topological superconductivity.

Prof. Fabien Bruneval
Service de Recherche en Métallurgie Physique, Gif-sur-Yvette, France
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Vertex corrections in MBPT_LCAO.

Dr. Jennifer Cano
Princeton University, New Jersey, USA
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Dr. Markus Ternes
Max Planck Institut für Festkörperforschung, Stuttgart, Germany
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Dr. Eric Bousquet
University of Liege, Belgique
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Prof. Elizabeth Pabón Gelves
Universidad Nacional de Colombia, Sede Medellin, Medellín-Antioquía, Colombia
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Dr. Adolfo G. Grushin
UC Berkeley / Néel Institute, University of California, USA
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Photogalvanic effect in chiral Weyl semimetals.

Dr. Francisco J. Terán
iMdea Nanociencia y Unidad Asociada al Centro Nacional de Biotecnología-CSIC, Madrid, Spain
28/08–28/08/2017
Probing the interaction of magnetic nanoparticles with biological entities by magnetic means.

Anna Oelsch
Johannes Kepler University, Linz, Austria
01/09–27/09/2017
Scanning Tunneling Microscopy, Low energy electron diffraction and photoemission experiments of boron doped graphene (B-Gr) and boron nitrate (BN) on curved Rhodium and Nickel substrates.

Dr. Ryoma Hayakawa
National Institute for Materials Science NIMS, Tsukuba, Japan
03/09–05/09/2017
Vertical resonant tunneling transistors with molecular quantum dots.

Prof. Walter Pfeiffer
University of Bielefeld, Germany
03/09–07/09/2017
Intra-atomic delays in attosecond time-resolved solid state photoemission.

Prof. Leonardo Marusic
University of Zadar, Croatia
04/09–09/09/2017
Electronic excitations in alkali-intercalated graphene.

Dr. Oleg Dolgov
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05/09–12/09/2017
Nature of superconducting glue and room-temperature superconductivity.

Prof. Archie Howie
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University of Cambridge, UK
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Comparison of photonics and fast electron interactions for plasmonics.

Prof. Rasmita Raval
University of Liverpool, UK
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Dr. Alessandro De Martino
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Monika Güttler
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Institut für Festkörperund Materialphysik, Dresden, Germany
09/09–17/09/2017
Compton scattering on 4f-systems.

Susanne Schulz
Technische Universität Dresden, Germany
09/09–17/09/2017
Design of 4f materials.

Prof. Magali Benoit
CEMES, Toulouse, France
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Dr. Paola Ferrario
Universidad de Valencia, Spain
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Dr. Giuseppe Foti
Institute of Physics, Czech Academy of Sciences, Czech Republic
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Current-induced heating and cooling dynamics in molecular junctions.

Dr. Anna Makarova
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Technische Universität Dresden, Germany
26/09–30/09/2017
Graphene and Boron nitride growth on curved surfaces.

Dr. Lucas Vazquez Besteiro
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Université du Québec, Varennes, Canada
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Chirality and plasmon particles.

Prof. Richard Korytár
Charles University, Prague, Czech Republic
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Quantum size effects in molecular wires and Kondo chains.

Prof. Ondrej Krivanek
Nion R&D, Arizona State University, Arizona, USA
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Vibrational spectroscopy in electron microscopy.

Prof. Marijan Sunjic
University of Zagreb, Croatia
03/10–31/10/2017
Dynamical response and surface excitations in thin films.

Prof. Daniel Jaque
Universidad Autónoma de Madrid, Spain
05/10–06/10/2017
Optical forces and torques at the nanoscale: Fundamentals and bio-applications.

Dr. Anton Tamtögl
Institute of Experimental Physics,
Graz University of Technology, Graz, Austria
10/10–19/10/2017
Surface diffusion and dynamics on Dirac materials.

Dr. Jonathan Bean
University of York, UK
15/10–21/10/2017
Electron transport in magnetic tunnel junctions.

Dr. Said Rahimzadeh-Kalaleh Rodriguez
AMOLF, Utrecht University, Holland
15/10–17/10/2017
Interacting photons.

Prof. Aristide Dogariu
CREOL, University of Florida, USA
21/10–20/11/2017
Optical interactions in complex media.

Prof. Juan José Gomez Cadenas
Instituto de Fisica Corpuscular CSIC-UV,
Valencia, Spain
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Dr. Yuan Zhang
Aarhus University, Aarhus, Denmark
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Prof. Francesc Monrabal Capilla
Texas A&M University, Texas, USA
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Prof. Annemarie Pucci
University of Heidelberg, Germany
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Prof. Albert Fert
UMR CNRS Thales, Palaiseau, France
27/10–30/10/2017
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Dr. Emmanuel Lassalle
Institute Fresnel, Marseille, France
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Dr. Xavier Monnier
University of Rouen Normandy, UFR Sciences et Techniques Technôpole du Madrillet,
Saint-Etienne du Rouvray, France
01/11–14/11/2017
Ultra-dense/low energy state glasses by aging nanostructured polymers.

Prof. Matteo Rizzi
Institut für Physik, Johannes Gutenberg Universität Mainz, Germany
07/11–12/11/2017
Topological insulators and quantum simulation in optical lattices.

Prof. María A. Díaz García
Universidad de Alicante, Spain
08/11–09/11/2017
Recent advances and new prospects on thin-film organic lasers.

Dr. Vladimir Zobac
Czech Academy of Sciences, Czech Technical Universityin Prague, Czech Republic
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Non-adiabatic molecular dynamics in molecular structures.

Dr. Yann Pouillon
Universidad de Santander, Spain
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Exact exchange and other new implementations within the SIESTA code.

Prof. Helmut Schwarz
Technische Universität Berlin, Germany
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The methane challenge C H Bond activation by metal oxides: theory and experiment in concert.

Dr. Fabio Pistolesi
Laboratoire Ondes et Matière d'Aquitaine,
Université Bordeaux & CNRS, France
13/11–14/11/2017
The bistability transition induced by a strong nano-electromechanical coupling.

Prof. H. Fabio Busnengo
Instituto de Fisica Rosario (CONICET-UNR) and Facultad Ciencias Exactas, Ingeniería y Agrimensura de la Universidad Nacional de Rosario, Argentina
16/11–20/11/2017
Gas surface dynamics and reactivity.

Prof. Álvaro De Rújula
IFT UAM-CSIC Madrid and CERN, Geneva, Switzerland
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Einstein's errors, triumphs and misconceptions.

Alice Lay
Stanford University, California, USA
19/11–23/11/2017
In vivo application of upconverting force sensors to elucidate neuromuscular pump action in c. elegans.

Prof. Kristján Leósson
Innovation Center, Iceland
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Dr. Marcelo Ciappina
ELI-Beamlines and Institute of Physics, Czech Academy of Sciences, Czech Republic
22/11–25/11/2017
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Dr. Lucian Constantin
Center for Biomolecular Nanotechnologies UNILE, Instituto Italiano di Tecnología, Arnesano, Italy
25/11–02/12/2017
Density functional theory development.

Prof. Antonio Acin
ICFO, Instituto de Ciencias Fotónicas, Castelldefels, Spain
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Dr. Vincenzo D'Ambrosio
ICFO, Castelldefels, Barcelona, Spain
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Eliska Greplova
Aarhus University, Denmark
03/12–08/12/2017
Fermionic gaussian channels.

Prof. Akio Kimura
Hiroshima University, Japan
03/12–08/12/2017
Topological insulators.

Dr. Mao Ye
Shanghai Institute of Microsystem and Information Technology, Chinese Academy of Sciences, China
03/12–08/12/2017
Topological insulators.

Dr. Iñigo Liberal Olleta
Universidad Pública de Navarra, Pamplona, Spain
05/12–05/12/2017
Light defies geometry in near-zero-index media.

Dr. Juan Carlos Idrobo
Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Tennessee, USA
17/12–20/12/2017
Electron energy loss spectroscopy of van der Waals heterostructures.

Dr. Pablo Lopez Tarifa
VU University Faculty of Sciences, Amsterdam, Netherlands
17/12–20/12/2017
SIESTA development: improvements in real-time TDDFT.

Dr. Alba Paniagua Diaz
University of Exeter, UK
17/12–18/12/2017
Wavefront shaping techniques to improve the detection of breast cancer.

Personnel

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Seminars

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20/12/2017
Dr. Jorge Luis Hita
Universidad Autónoma de Madrid, Spain

2 What we gain with aberration-correctors and monochromators — probing bonding, magnetism, temperature & an harmonicity at the nanoscale
19/12/2017
Juan Carlos Idrobo
Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, USA

3 Wavefront shaping techniques to improve the detection of breast cancer
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Alba Paniagua-Diaz
Physics and Astronomy, University of Exeter, UK

4 Light defies geometry in near-zero-index media
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Universidad Pública de Navarra, Spain

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Eliska Greplova
Aarhus University, Denmark

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ICFO, Instituto de Ciencias Fotónicas, Castelldefels, Spain

7 Attosecond physics at the nanoscale: the next frontier
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Dr. Marcelo Ciappina
ELI-Beamlines and Institute of Physics, Czech Academy of Sciences, Czech Republic

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Dr. Magdalena Marganska-Lyzniak
Universität Regensburg, Institute for Theoretical Physics, Germany

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Stanford University, California, USA

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Saint Petersburg State University, St. Petersburg, Russia

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Service de Recherche en Métallurgie Physique, Gif-sur-Yvette, France

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Centre de physique théorique, Université Aix-Marseille, France

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From organic semiconductors to 2d layered materials
06/04/2017
Prof. Thomas Weitz
AG Physics of Nanosystems, LMU Munich, Germany

55 Molecular magnetic coolers
24/03/2017
Dr. Marco Evangelisti Crespo
CSIC, Instituto de Ciencia de Materiales de Aragón, Universidad de Zaragoza, Spain

56 Tensor networks for quantum matter: basics, news and prospects
17/03/2017
Prof. Román Orús Lacort
Johannes Gutenberg-Universität Mainz, Germany

57 Enabling sensing technology with plasmonics
16/03/2017
Prof. François Lagugné-Labarthet
Western University, London, Ontario, Canada

58 Testing many-body world with a few strongly correlated ultra-cold fermions
02/03/2017
Prof. Tomasz Sowinski
Quantum Optics Group, Institute of Physics of the Polish Academy of Sciences, Warsaw, Poland

59 The Nobel Prize 2016: topology in nonrelativistic quantum mechanics
24/02/2017
Prof. Raffaele Resta
Università di Trieste, Italy

60 Weyl fermions from crystal symmetry
17/02/2017
Prof. Juan Luis Mañes
Facultad de Ciencia y Tecnología, UPV/EHU, Leioa, Spain

61 Charge transport: from Faraday to Thouless
10/02/2017
Prof. Raffaele Resta
Università di Trieste, Italy

62 Spontaneous natural optical activity in disordered media
06/02/2017
Prof. Felipe Pinheiro
Federal University of Rio de Janeiro, Brazil & Optoelectronics Research Centre, Southampton, UK

63 The knowledge and innovation community on raw materials
02/02/2017
Dr. Serge Monturet
EIT RawMaterials CLC Central, Metz, France

64 Topological chemistry
27/01/2017
Prof. Bogdan Andrei Bernevig
Princeton University, New Jersey, USA

65 On-surface synthesis and properties characterization of novel low-dimensional materials
25/01/2017
Dr. Oliver Gröning
EMPA, Switzerland

66 Giant edge spin accumulation in a symmetric quantum well with two subbands
19/01/2017
Prof. Alexander Khaetskii
University at Buffalo, New York, USA

Workshops

Ether and Modernity. The Recalcitrance of an Agonising Object in Physics and in Culture

March 30-31, 2017
DIPC, Donostia / San Sebastián
https://www.ehu.eus/en/web/etherandmodernity

Organizer
Prof. Jaume Navarro (DIPC, UPV/EHU)

Physicists, Historians of Science and Philosophers were invited to attend and submit short presentations to the workshop "Ether and Modernity", on the presence of the ether in twentieth century science and culture.

This was the third of a series of meetings (Oxford 2014, San Francisco 2015, San Sebastian 2017) to discuss the way an epistemic object like the ether was rejected, modified or maintained in the first half of the twentieth century, and the later attempts to resuscitate it in contemporary physics. The workshop had a twofold practical purpose: the finalisation of a joint publication with the contributions of the invited speakers; and the dissemination of the results and the incorporation of new ideas into the project by other historians of science, physicists and philosophers.

Invited Speakers
Imogen Clarke (Independent Scholar)
Connemara Doran (Harvard University)
Linda D. Henderson (University of Texas)
Roberto Lalli (Max Planck Institute for the History of Science)
Jaume Navarro (Ikerbasque and University of the Basque Country)
Richard Noakes (University of Exeter)
Arne Schirrmacher (Humboldt University)
Richard Staley (University of Cambridge)
Scott A. Walter (University of Nantes)
Michael Whitworth (University of Oxford)
Aaron Wright (Stanford University)

13th Capri Spring School on Transport in Nanostructures 2017

April 23-30, 2017
Villa Orlandi, Isola di Capri, Italy
http://www.capri-school.eu/capri17/

Organizing Committee
Dario Bercioux (Ikerbasque, DIPC)
Alessandro De Martino (City, University of 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 spring school provided lectures by leading experts supplemented by a few shorter seminars. The 2017 school addressed solid-state quantum information processing. The speakers gave graduate level presentations introducing to state-of-the-art methods and techniques featuring the key issues of the field of solid-state quantum information processing. While the school was primarily aimed at instructing PhD students and young postdoctoral researchers, more senior scientists who wanted to acquaint themselves with the subject of the school were also welcome.

Invited Speakers
Alexander Altland (Cologne)
Jens Eisert (Berlin)
Andrew Cleland (Chicago)
Daniel Loss (Basel)
Michel H. Devoret (Yale)
Enrique Solano (Bilbao)
David P. DiVincenzo (Aachen)

Discussions on Nano & Mesoscopic Optics (DINAMO-2017)

May 14-19, 2017
Siglufjordur, Iceland
http://dinamo2017.nmi.is

Organizing Committee
Andrea Bragas (CONICET, UBA, Argentina)
Kristján Leósson (Innovation Center Iceland)
Stefan A. Maier (Imperial College London, UK)
Juan José Sáenz (DIPC, Donostia / San Sebastián, Spain)

Local Committee
Sigridur Ingvarsdottir (Innovation Center Iceland)
Fjalar Sigurdarson (Innovation Center Iceland)

International Scientific Committee
Javier Aizpurua (DIPC, Donostia / San Sebastián, Spain)
Gabriel Cwilich (Yeshiva University, New York, USA)
Aristide Dogariu (CREOL, Florida, USA)
F.J. García-Vidal (IFIMAC-UAM, Madrid, Spain)
Lukas Novotny (ETH-Zürich, Switzerland)
Markus Schmidt (IPHT Jena, Germany)
Fernando Stefani (CONICET, UBA, Argentina)

Nano and Mesoscopic Optics involves the interaction of light with structures that are too small or too complex to be described by traditional continuum methods, as well as the structuring and manipulation of optical fields and interactions at sub-wavelength scale. This is a highly active and interdisciplinary area of research which involves experimental and theoretical experts from optics, acoustics, biophysics, cold atom and condensed matter physics, and telecommunications.

DINAMO promotes the transfer of knowledge between different branches of science and stimulate a global solutions to complex problems of nano and mesoscopic optics. DINAMO is conceived to provide an interdisciplinary forum where leading investigators from around the world can present and discuss their latest work and future challenges in an informal and interactive format.

Beautiful natural locations and isolated venues promote the scientific and personal interaction during presentations, discussion, meals, outdoor excursions and social events. The first DINAMO conference was held in "El Chalten" in Patagonia, Argentina in 2015. In 2017, a new remote location will offer an exceptional environment for the second meeting in the series.

Invited Speakers
Guillermo Acuña (TU Braunschweig, Germany)
Paloma Arroyo-Huidobro (Imperial College London, UK)
Markus Aspelmeyer (University of Vienna)
Jacobo Bertolotti (University of Exeter, UK)
Nicolas Bonod (Fresnel, Marseille, France)
Sergey Bozhevolnyi Syddansk Universitet, Denmark)
Andrea Bragas (Universidad de Buenos Aires)
Hui Cao (Yale University)
Remi Carminati (Institut Langevin, ESPCI, Paris)
Emiliano Cortes (Imperial College London)
Gabriel Cwilich (Yeshiva University, New York)
Javier García de Abajo (ICFO, Barcelona)
Antonio García-Martin (IMM, CSIC, Madrid)
Simone De Liberato (University of Southampton)
Thomas Dekorsy (DLR Stuttgart, Germany)
Aristide Dogariu (CREOL, Florida)
Johannes Feist (IFIMAX, Universidad Autónoma de Madrid)
Jochen Feldmann (LMU Munich)
Mathias Fink (Institut Langevin, ESPCI, Paris)
Ernst-Ludwing Florin (University of Texas at Austin)
Martin Frimmer (ETH, Zurich, Switzerland)
Luis Froufe-Perez (Université de Fribourg, Switzerland)
Aitzol Garcia-Etxarri (DIPC, Donostia / San Sebastián)
Harald Giessen (Stuttgart University)
Sylvain Gigan (Ecole Normale Sup., Paris)
Rainer Hillenbrand (CIC nanoGUNE, Donostia / San Sebastián, Spain)
Mikael Käll (Chalmers, Gothenburg)
Arseniy Kuznetsov (DSI, Singapore)
Daniel Lanzillotti-Kimura (CNRS, Université Paris-Sud)
Kristján Leósson (Innovation Center Iceland)
Cefe Lopez (ICMM-CSIC, Madrid)
Stefan Maier (Imperial College London)
Andrei Manolescu (Reykjavik University)
Onofrio Marago (Messina, Italy)
Manuel Marques (IFIMAC-UAM, Madrid)
Otto Muskens (University of Southampton)
Michel Orrit (University of Leiden)
Helmut Ritsch (University of Innsbruck)
Monika Ritsch-Marte (Medical University Innsbruck, Biomedical Physics)
Halina Rubinsztein-Dunlop (University Queensland, Australia)
Juan José Sáenz (DIPC, Donostia-San Sebastian)
Jose Sanches-Gil (IEM, CSIC, Madrid)
Riccardo Sapienza (King College London)
Frank Scheffold (Université de Fribourg, Switzerland)
Markus Schmidt (University Jena)
Fernando Stefani (CIBION, Buenos Aires)
Philip Tinnefeld (TU Braunschweig)
Agust Valfells (Reykjavik University)
Niek van Hulst (ICFO, Barcelona)
Silvia Vignolini (University of Cambridge, UK)
Giorgio Volpe (University College London, UK)
Giovanni Volpe (University of Gothenburg, Sweden)
Pavel Zemanek (ISI, Czech Academy of Sciences)

From Bioinorganic Chemistry to Catalysis

June 6, 2017
Faculty of Chemistry, UPV/EHU , Donostia / San Sebastián
http://dipc.ehu.es/ws_presentacion.php?id=160

Organizing Committee
Zoraida Freixa (Ikerbasque, UPV/EHU, Spain)
Luca Salassa (Ikerbasque, DIPC, Spain)
Miguel Huertos (Ikerbasque, UPV/EHU, Spain)
Jon M. Matxain (UPV/EHU – DIPC, Spain)
Eider San Sebastián (UPV/EHU, Spain)

This one-day workshop brought together researchers active in the interconnected fields of molecular catalysis and bioinorganic chemistry, targeting an audience of young master and doctorate students. The aim of the meeting was to create new synergies among researchers working in various research institutes located in Donostia. The workshop also counted with the kind participation of invited scientists coming from IMDEA Nanociencia and the University of Vienna.

Invited speakers
Ana M. Pizarro (IMDEA Nanociencia, Spain)
Alessio Terenzi (University of Vienna, Austria)
Marek Grzelczak (Ikerbasque, CIC biomaGUNE, Spain)
Xabi Lopez (UPV/EHU – DIPC, Spain)
Jon M. Matxain (UPV/EHU – DIPC, Spain)
Arkaitz Correa (UPV/EHU, Spain)
Torrent-Sucarrat Miquel (Ikerbasque, UPV/EHU – DIPC, Spain)
Hartiz Sardon (Ikerbasque, UPV/EHU – POLYMAT, Spain)
Fernando López-Gallego (Ikerbasque, CIC biomaGUNE, Spain)
Zoraida Freixa (Ikerbasque, UPV/EHU, Spain)
Luca Salassa (Ikerbasque, DIPC, Spain)
Miguel Huertos (Ikerbasque, UPV/EHU, Spain)

HPC Knowledge Meeting '17

June 15-16, 2017
Miramar Palace, Donostia / San Sebastián
http://hpckp.org/index.php/annual-meeting/hpckp-17

The global conference HPC Knowledge Meeting '17 was aimed at sharing expertise and strategies in High Performance Computing, High Performance Data Analysis and Clustering. Some of the most skilled HPC professionals from all over the world were called to be present in this annual meeting where new trending topics and innovations in the HPC world are exposed and discussed with this distinguished public.

The HPCKP project was founded in late 2010 as an initiative of The Reference Network on Theoretical and Computational Chemistry (XRQTC), with the idea of sharing the deep knowledge acquired by people in the HPC field regarding installation and optimization of specific applications in Computational Chemistry. The project has rapidly became an international reference covering several scientific domains.

Since 22 March 2013, HPCNow! supports and manages the HPC Knowledge Portal. HPCNow! was born as a natural evolution of the HPCKP project, and ensures the continuity and sustainability of the HPC Knowledge Portal.

Invited speakers
Rob Farber (TechEnablement.com)
Ingrid Barcena (KU Leuven)
Hussein N. Harake (CSCS)
Todd Gamblin (LLNL)
Robert McLay (TACC)
Kenneth Hoste (Ghent University)
Jordi Blasco (HPCNow!/NeSI)
Rosa Filgueira (British Geological Survey, NERC, Edinburgh, UK)
Judit Gimenez (BSC)
Adam Roe (Intel Corporation)
Albert Valls (IBM)
Carles Fenoy (Roche)
Andrés Díaz-Gil (IFT-CSIC)
Alejandro Sanchez (SchedMD)
Luigi Brochard (Lenovo)
Shahzeb Siddiqui (Pfizer)

13th European Conference on Surface Crystallography and Dynamics (ECSCD-13)

June 19-21, 2017
Miramar Palace, Donostia / San Sebastián
http://ecscd13.dipc.org/

Organizing Committee
María Blanco-Rey (UPV/EHU)
Martina Corso (CFM-CSIC-UPV/EHU
Aran García-Lekue (DIPC)
Celia Rogero (CFM-CSIC-UPV/EHU)
Karmela Alonso Arreche (DIPC)

Scientific Committee
María Blanco-Rey (Universidad del País Vasco UPV/EHU, San Sebastián, Spain)
Giovanni Comelli (University of Trieste; IOM CNR, TASC Lab., Italy)
Ulrike Diebold (Technische Universität Wien, Austria)
Juan de la Figuera (Instituto de Química Física Rocasolano, CSIC, Madrid, Spain)
Axel Groß (Universität Ulm, Germany)
Georg Held (University of Reading, UK)
Pavel Jelinek (Institute of Physics, Czech Academy of Science, Prague, CZ)
Edvin Lundgren (University of Lund, Lund, Sweden)
Katariina Pussi (Lappeenranta University of Technology, Finland)
Karsten Reuter (chair), Technische Universität München, Germany)
Philippe Sautet (CNRS and Ecole Normale Supérieure of Lyon, France)
Hans-Peter Steinrück (Universität Erlangen-Nürnberg, Germany)
Stefan Tautz (Peter Grünberg Institute, Forschungszentrum Jülich, Germany)
D. Phil Woodruff (University of Warwick, UK)
Harold J.W. Zandvliet (University of Twente, Netherlands)

The European Conference on Surface Crystallography and Dynamics (ECSCD) is aimed at discussing the recent advances on the characterization of dynamical processes and structure of surfaces, as well as their interplay, at the atomic length scale. The first edition of the conference took place in 1985 in Erlangen (Germany), and it has become a well established meeting point for the surface science community. In its 13th edition, it will tackle two-dimensional materials, single molecules on surfaces, characterization by LEEM and PEEM, oxides, and other representative topics of present-day surface science. Following the ECSCD tradition, networking between experimentalists and theoreticians will be encouraged, bringing together experienced and young researchers working in the field.

Keynote Speakers
Andrea Locatelli (Elettra Sincrotrone Trieste, Italy)
Jascha Repp (Faculty of Physics, University of Regensburg, Germany)
Daniel Sánchez-Portal (Centro de Física de Materiales CFM/MPC (CSIC-UPV/EHU), Donostia-San Sebastián, Spain)

Invited Speakers
Lucía Aballe (ALBA Synchrotron, Barcelona, Spain)
Cristina Africh (Istituto Officina dei Materiali, CNR-IOM, Trieste, Italy)
Andrey Chuvilin (CIC nanoGUNE, Donostia-San Sebastián, Spain)
Stefan Förster (Martin Luther Universität, Halle-Wittenberg, Germany)
Silvia Gallego (Instituto de Ciencia de Materiales de Madrid, CSIC, Spain)
Andrew Gellman (Chemical Engineering Faculty, Carnegie Mellon University, USA)
Jeppe V. Lauritsen (Interdisciplinary Nanoscience Center, Aarhus, Denmark)
Jorge Lobo-Checa (Instituto de Ciencia de Materiales de Aragón CSIC, Zaragoza, Spain)
Olaf Magnussen (Christian-Albrechts-Universität zu Kiel, Germany)
Philip Moriarty (School of Physics and Astronomy, University of Nottingham, UK)
Tomoko Shimizu (National Institute of Materials Science, Tsukuba, Japan)
Marialore Sulpizi (Institute of Physics, Johannes Gutenberg Universität, Mainz, Germany)
Charles Sykes (Department of Chemistry, Tufts University, USA)

8th International Theoretical Biophysics Symposium (THEOBIO 2017)

June 26-230, 2017
Miramar Palace, Donostia / San Sebastián
http://theobio17.dipc.org/

Organizing Committee
Xabier Lopez (UPV/EHU)
Elixabete Rezabal (UPV/EHU)
Elena Formoso (UPV/EHU)
Jon I. Mujika (DIPC)
Rafael Grande-Aztatzi (DIPC)

International Committee:
Carlo Adamo (ENSCP – Chimie ParisTech, France)
Leif A. Eriksson (University of Gothenburg, Sweden)
Maria Joao Ramos (University of Porto, Portugal)
Francesca Mocci (University of Cagliari, Italy)
Nino Russo (University of Calabria, Italy)
Xabier Lopez (UPV/EHU)
Jesus Ugalde (UPV/EHU)

This International Conference focused on state-of-the-art methods and applications on the computational modeling of biochemical and biophysical systems, comprising from all-atom highly accurate electronic structure calculations to the simulation of mesoscopic systems with coarse-grained method. Both methodological developments and applications were welcome.

Plenary Speakers
Anna Peacock (University of Birmingham)
Darrin M. York (Rutgers University, New Jersey)
Felix Goñi (University of the Basque Country and Basque Centre for Biophysics)
Pedro A. Fernandes (Universidade do Porto)
Paolo Carloni (Institute for Advanced Simulations, Jülich)
Oscar Millet (CIC bioGUNE, Derio)
Silvia Osuna (Universitat de Girona)

Invited Speakers
Elena Formoso
Francesca Mocci
Iñaki Tuñon
Irene Maffucci
Jitrayut Jitonnom
Jaroslav Burda
Jon I. Mujika
José Pedro Cerón-Carrasco
Kwangho Nam
Leif A. Eriksson
Maria João Ramos
Marta Alberto
Natacha Gillet
Nikolay Blinov
Olalla Nieto
Ran Friedman
Sara Capponi
Serdar Durdagi

Software Carpentry

June 28-30, 2017
Elbira Zipitria Center UPV/EHU, Donostia / San Sebastián
http://iamc.eu/2017-06-28-cfmehu/

Organizing Committee
Iñigo Aldazabal Mensa (CFM (CSIC-UPV/EHU))
Andrés Diaz-Gil (Instituto de Física Teórica (CSIC-UAM), Madrid)
Mateusz Kuzak (Netherlands eScience Center, Amsterdam)

Helpers
Unai Aseguinolaza, Tineke van den Berg, Brendan Costello, Daniel Franco, Diego Lasa, Irene Monsalve, Sanjeev Nara, David de Sancho, Camila Zugarramurdi

Software Carpentry aims to help researchers get their work done in less time and with less pain by teaching them basic research computing skills. This hands-on workshop will cover basic concepts and tools, including program design, version control, data management, and task automation. Participants will be encouraged to help one another and to apply what they have learned to their own research problems.

Syllabus
The Unix Shell
Programming with Python
Version Control with Git
Introduction to Scientific Python

Frontiers in Quantum Materials and Devices (FQMD)

July 13-14, 2017
Miramar Palace, Donostia / San Sebastián
http://ciqm.harvard.edu/fqmd-2017-frontiers-in-quantum-materials-and-devices.html

Organizing Committee
Vitaly Golovach (Ikerbasque, CFM and DIPC)
Naomi Brave (Harvard University)
Robert Westervelt (Harvard University)
Daniel Loss (University of Basel)

DIPC organized jointly with Harvard University the international conference Frontiers in Quantum Materials and Devices (FQMD). The workshop focused on exciting discoveries in Atomic-scale Electronics, Photonics, and Quantum Information Science. Quantum materials offer dramatically new approaches for electronics and photonics, but their characteristics, and the techniques to make devices and interconnected systems are largely unknown. The Frontiers in Quantum Materials and Devices workshops addressed this challenge by bringing together experts in materials growth and characterization, device fabrication and testing, and theoretical modeling. Through interactive talks and discussions, they were able to develop the science and technology needed to advance the science and move toward applications.

Invited Speakers
Tomasso Calarco (Institute of Complex Quantum Systems, Ulm University)
Yoshinori Tokura (Center for Emergent Matter Science RIKEN & University of Tokyo)
Leo Kouwenhoven (Microsoft Station Q and QuTech, Delft University of Technology)
Vidya Madhavan (University of Illinois at Urbana-Champaign)
Seigo Tarucha (University of Tokyo and Center for Emergent Matter Science RIKEN)
Jelena Klinovaja (University of Basel)
Andras Kis (École Polytechnique Fédérale de Lausanne)
Deji Akinwande (University of Texas, Austin)
Masashi Kawasaki (Center for Emergent Matter Science RIKEN & University of Tokyo)
Claudia Felser (Max Planck Institute of Chemical Physics for Solids)
James Analytis (University of California, Berkeley)
Pablo Jarillo-Herrero (Massachusetts Institute of Technology)
Marko Loncar (Harvard University)
Liam McGuinness (Institute for Quantum Optics, Ulm University)
Florian Marquardt (Max Planck Institute for the Science of Light)
Javier Aizpurua (Ctr for Materials Physics & Donostia International Physics Ctr)
Yoshiro Hirayama (Tohoku University)

Nanophotonics of 2D materials, N2D 2017

July 31 - August 3, 2017
Miramar Palace, Donostia / San Sebastián
http://n2d.dipc.org/

Organizing Committee
Alexey Nikitin (CIC nanogune, Spain)
Luis Martín-Moreno (ICMA, CSIC Zaragoza, Spain)
Tony Low (University of Minnesota, USA)

Over the past decade, there is a growing research activity on light-matter interactions in atomically thin materials, such as graphene, topological insulators, thin polar and semiconducting layers and other van der Waals materials, including their heterostructures. Nanophotonics of 2D materials (N2D) aims at the exploration of their optical phenomena and in providing a setting where researchers from diverse fields can convene; classical and quantum optics; excitons, phonons and plasmons; far-field and near field spectroscopies; many body optical physics; topological photonics; among many others. Through these interactions, N2D seeks to provide a setting where unifying concepts can form, new ideas inspired, and new frontiers in theoretical and experimental research on 2D materials nanophotonics can emerge.

Invited Speakers
Rainer Hillenbrand (CIC nanoGUNE, Spain)
Mark Rudner (Niels Bohr Institute, Denmark)
Alexey Kuzmenko (Université de Genève, Switzerland)
Gilbert Walker (University of Toronto, Canada)
Javier Garcia de Abajo (ICFO, Spain)
Tony Heinz (Stanford University, USA)
Alexander Grigorenko (University of Manchester, UK)
Andres Castellanos-Gomez (IMDEA, Spain)
Zubin Jacob (Purdue University, USA)
Atac Imamoglu (ETH Zurich, Switzerland)
Sang-Hyun Oh (University of Minnesota, USA)
Stefano Lupi (Sapienza Università di Roma, Italy)
Joshua Caldwell (U.S. Naval Research Laboratory, USA)
Pablo Alonso González (Universidad de Oviedo, Spain)
Grace Xing (University of Notre Dame, USA)
Marco Polini (IIT, Italy)
Ido Kaminer (MIT, USA)
Nuno Peres (Universidade do Minho, Portugal)
Stéphane Kéna-Cohen (Polytechique Montréal, Canada)
Frank Koppens (ICFO, Spain)
Thomas Taubner (U. RWTH Aachen, Germany)
Cyriaque Genet (U. Strasbourg, France)
James Hone (Columbia University, USA)
Chee Wei Wong (University of California, USA)
Lifa Zhang (University of Nanjing, China)
Jorge Cuadra (Chalmers, Sweden)
Michael Fogler (University of San Diego, USA)
Nathaniel Gabor (University of California, USA)
Roman Krahne (IIT, Italy)
Pablo Merino (ICMM, Spain)
Tobias Stauber (ICMM, Spain)
Yuriy Zakharko (University of Heidelberg, Germany)

Quantum Spintronics at Interfaces (Magnon)

September 4-8, 2017
Miramar Palace, Donostia / San Sebastián
http://magnon.dipc.org/

Organizing Committee
Yaroslav Tserkovnyak (University of California, USA)
Vitaly Golovach (CFM CSIC-UPV/EHU and DIPC)
Sebastian Bergeret (CFM CSIC-UPV/EHU and DIPC)
Tineke van den Berg (CFM CSIC)

The workshop focused on novel phenomena occurring at interfaces between metallic conductors and magnetic insulators, including new classes of quantum magnetic materials, which offer a rich playground for Quantum Spintronics. The workshop will bring together leading experts, experimentalists and theorists, working at the crossroads between magnon spintronics and quantum magnetism. We will discuss recent developments in electrical control and detection of spin currents through magnetic insulators, collective spin transport and spin waves, quantum correlations and novel quantum heterostructures for spintronics, bosonic condensation and superfluidity of magnons, topological order and dynamics in quantum magnetic materials. We hope the workshop will foster collaborations in this rapidly developing field, important for the fundamental physics and applications.

Invited Speakers
Christian Back (Regensburg)
Gerrit Bauer (Sendai)
Miguel A. Cazalilla (Hsinchu)
Irene D'Amico (University of York)
Rembert Duine (Utrecht)
Michael Flatté (Iowa)
Benedetta Flebus (Utrecht)
Pietro Gambardella (Zürich)
Francisco Guinea (Madrid/Manchester)
Wei Han (Beijing)
Ewelina Hankiewicz (Würzburg)
Daichi Hirobe (Tohoku)
Mathias Kläui (Mainz)
Takis Kontos (Paris ENS)
Daniel Loss (University of Basel)
Allan MacDonald (UT Austin)
Hector Ochoa (UCLA)
Yoshichika Otani (Tokyo)
Ignacio Pascual (Donostia)
Marco Polini (IIT)
Roberto Raimondi (Univ of Roma Tre)
Christian Rüegg (PSI Villigen)
Nitin Samarth (Penn State)
Eugene Sherman (Bilbao)
Masashi Shiraishi (Kyoto Univ)
Jairo Sinova (Mainz)
Ilya Tokatly (Donostia)
Saul Velez (Donostia)
Giovanni Vignale (Univ of Missouri)
Roland Winkler (Northern Illinois University)
Dominik Zumbühl (Basel)

Summer School

Frontiers of Condensed Matter

September 18-29, 2017
Casimir Research School, Les Houches, France
https://casimir.researchschool.nl/summer-school-les-houches-france-frontiers-of-condensed-matter-3203.html

Organizing Committee
Sebastien Bergeret (DIPC, CFM/CSIC, Spain)
Julia Meyer (Université Grenoble Alpes, France)
Tjerk Oosterkamp (Leiden Institute of Physics, Netherlands and Casimir Research School)

This Les Houches international doctoral training session aims at offering Master and PhD students a training program in the area of Condensed Matter Physics. It was organized jointly by the Ecole Doctorale de Physique de Grenoble (France), the Casimir Research School Delft-Leiden (Netherlands), and the Donostia International Physics Center, San Sebastian (Spain).

The program consisted of several courses. The courses were complemented by more specialized research seminars on timely topics. During the sessions, there was time for informal discussions between participants and lecturers. A poster session was organized, including a short oral presentation at the beginning of the sessions enabling the participants to present their research interests to each other.

Invited Speakers
Y. Nazarov (Delft & "Chaire d'excellence" Grenoble)
M. Houzet (Grenoble)
Roman Orus (Mainz)
G. Steele (Delft)
J. Pekola (Aalto & "Chaire d'excellence" Grenoble)
L. Fritz (Utrecht)

Exotic New States in Superconducting Devices: The Age of the Interface

September 25-28th 2017
Mainz, Germany
https://www.spice.uni-mainz.de/ens-workshop-2017-home/

Organizing Committee
Sebastian Bergeret (CSIC/DIPC)
Jason Robinson (University of Cambridge)
Kjetil Hals (JGU Mainz)

At the interface between a superconductor and a non-superconducting material such as a ferromagnet, a topological insulator or a semiconductor, a range of electronic states can be induced which are radically different from either constituent material. To be able to probe these states requires a broad range of expertise, spanning basic materials science to fundamental physics modeling of interfaces and transport behaviour.

At this meeting we had the opportunity to bring together scientists working on distinct and overlapping areas, such as superconductivity, magnetism, topological materials, quantum computing, and spin-electronics. This science community enjoyed how these different transport phenomena are linked conceptually and thereby stimulate further understanding particularly with respect to realising useful devices with unique properties for spin-electronics and quantum computing.

Invited Speakers
Jan Aarts (University of Leiden)
Marco Aprili (CNRS-Paris)
Norman Birge (Michigan State University)
Mark Blamire (University of Cambridge)
Silvano De Franceschi (CEA Grenoble)
Matthias Eschrig (Royal Holloway, London)
Mikael Fogelström (Chalmers)
Katharina Franke (Freie Universität Berlin)
Francesco Giazotto (CNR-Pisa)
Sophie Gueron (LPS-Orsay)
Ewelina Hankiewicz (Würzburg Univ.)
Tero Heikkilä (University of Jyväskylä)
Leo Kouwenhoven (Delft)
Yoshi Maeno (University of Kyoto)
Dirk Manske (MPI-Stuttgart)
Julia Meyer (CEA Grenoble)
Oded Millo (University of Jerusalem)
Jagadeesh Moodera (MIT)
Stuart Parkin (MPI, Halle)
Dimitri Roditchev (INSP Paris)
Ilya Tokatly (University of Basque Country)
Javier Villegas (CNRS-Thales)
Felix von Oppen (FU Berlin)

Iberian Vacuum Conference, RIVA-X

October 4-6, 2017
Bilbao, Spain

Organizing Committee
J. Barriga (Tekniker)
E. Ortega (UPV/EHU, DIPC, CFM)
J.A. Martín-Gago (Institute of Materials Science of Madrid-CSIC)
M.F. López (Institute of Materials Science of Madrid-CSIC)
A. López Vazquez de Parga (UAM)
F. Tabarés (CIEMAT)
Carlos Jose Tavares

The Iberian Vacuum Conference, RIVA is a joint meeting of the Spanish Vacuum Society (ASEVA) and the Portuguese Vacuum Society (SOPORVAC), and follows the series started in Braga, Portugal, in 1988, changing alternative the location between Portugal and Spain. The main goal of this conference is to cover the fields of vacuum and its applications, particularly on the fields of Fundamental and Applied Surface Science, Thin Films, Electronics Materials and Processing, Plasma physics, Vacuum Science and technology and Nanometer Scale processes.

The Conference provided a forum where the most relevant and recent results were discussed. We invited scientists and engineers from Spain and Portugal, as well as those from other countries, who took part in this event, especially junior ones.

8th European Topical Conference on Hard Coatings
One of the sessions within Riva-X was devoted to hard coating.

Plenary Speakers
Prof. Lars Montelius (Director General INL, PT)
Prof. Peter J Kelly (Manchester Metropolitan University, UK)
Prof. Marek Rubel (Royal Institute of Technology (KTH), SE)
Dr. Ibon Bustinduy Uriarte (European Spallation Neutron Source Bilbao (ESS), ES)

Invited Speakers
Prof. Osvaldo de Melo (Universidad de La Habana, Cuba)
Prof. Clemens Laubschat (Technische Universität Dresden, DE)
Dr. Carlo Morasso (Laboratory of Nanomedicine and Clinical Biophotonics, IT)
Prof. Tomas Polcar (University of Southampton, UK)
Prof. Jose Ignacio Pascual (Nanogune, ES)
Pedro Salomé (Iberian Nanotechnology Laboratory, INL, PT)
Dr. Michael Foerster (ALBA synchrotron, ES)
Dr. Otmar Zimmer (Fraunhofer IWS, DE)

Yáñez Workshop

October 26, 2017
DIPC, Donostia / San Sebastián

Organizing Committee
Jesus M. Ugalde
Begoña Lecea
Fernando Castaño
Pascual Román
Luis Laín
Alicia Torre
Teófilo Rojo

The Yáñez Workshop, dedicated to the life-time achievements of Prof. Manuel Yáñez, was held on the occasion of the Doctor Honoris Causa Award presentation ceremony to Profs. Manuel Yáñez and Albert Fert. The Yáñez Workshop consisted of 12 lectures arranged in four session. The speakers addressed an professional audience however not necessarily experts on the themes of talks. The audience included colleagues as well as friends of Prof. Manuel Yáñez.

Invited Speakers
Venancio Pardo
David de Sancho
Fernando Martin
Elena Formoso
Antonio Largo
Fernando Ruiperez
Gernot Frenking
Enrique Orti
Leticia Gonzalez
David Casanova
Jeremy Harvey
Angel M. Pendas
Ibon Alkorta
Mario Piris
Mariona Sodupe
J. Andres Fernandez
Arvi Rauk

Emergence: Epistemological and Metaphysical Issues

October 26-27 2017
DIPC, Donostia / San Sebastián
http://www.ehu.eus/ehusfera/ink/eemi17/

Organizing Committee
Javier Cumpa (Universidad de Complutense de Madrid)
Andoni Ibarra (UPV/EHU)
Thomas Mormann (UPV/EHU)
Jaume Navarro (UPV/EHU Ikerbasque)
Iñaki San Pedro (UPV/EHU)

Scientific Committee
Otávio Bueno (Miami)
Javier Cumpa (Universidad de Complutense de Madrid)
Iñaki San Pedro (UPV/EHU)
Jessica Wilson (Toronto)

The aim of the workshop was to discuss issues concerning emergence, ranging from epistemological issues related to the emergence of properties in specific scientific practices —such as physics, computer science or climate change— to metaphysical issues in connection with the nature and ontology of emergent properties.

Invited Speakers
Mark A. Bedau (Reed)
Otávio Bueno (Miami)
Javier Cumpa (U. Complutense Madrid)
Álvaro de Rújula (CERN)
Robin Hendry (Durham)
Paul Humpreys (Virginia)
Iñaki San Pedro (UPV/EHU)
Ferdinando Villa (BC3)
Jessica Wilson (Toronto)

Modern Trends in Molecular Dynamics and Electron Correlations at Surfaces and Interfaces

October 27, 2017
Miramar Palace, Donostia / San Sebastián
http://modsurf.dipc.org/

Organizing Committee
Denis Vyalikh (DIPC)
Ricardo Díez Muiño (DIPC and CFM, CSIC-UPV/EHU)
Clemens Laubschat (Technische Universität Dresden)

The program of the workshop included recent examples of research performed in collaboration between groups at Donostia International Physics Center (DIPC) and groups at different German universities. DIPC is a research center whose main goal is to perform and catalyze cutting-edge research in physics and related disciplines, as well as to convey scientific culture to society. DIPC is an international research center, a hub between the local community of scientists and a world-wide network of researchers from other institutions. For this purpose, DIPC holds a strong program of visiting scientists that has brought 2750 visitors to the Center in the period 2000-2016. In this international effort, German research groups have historically played a major role. Germany is the top country in the number of joint publications with DIPC researchers, with 680 articles, as of August 2017.

There are currently several research projects going on that involve scientific collaboration between DIPC groups and German groups at the forefront of research in the fields of condensed matter physics, surface science, and nanoscience, among others. The scientific program of the workshop "Modern Trends in Molecular Dynamics and Electron Correlations at Surfaces and Interfaces" provided an overview of some of these projects, including recent results. The workshop also served as a meeting point for scientists. Future funding opportunities were discussed as well.

Invited Speakers
Ricardo Díez Muiño
Clemens Laubschat
Michael Mößle
Adolfo Morais
Javier Aizpurua
Annemarie Pucci
Björn Trauzettel
F. Sebastián Bergeret
Eugene Krasovskii
Jan Ingo Flege
Denis Vyalikh
Yoav William Windsor
J. Enrique Ortega Anna Makarova
Peter Saalfrank
Iñaki Juaristi
Maite Alducin
Rolf Möller
Nicolás Lorente
Ulrich Höfer
Frederik M. Schiller
Eugene V. Chulkov
Laura Fernández
María Blanco-Rey

Higher Education

DIPC School

Surfaces and Interfaces

June 20-23, 2017
Miramar Palace, Donostia / San Sebastián
http://www.nanogune.eu/event/sschool2017

Chairman
Jose M. Pitarke (CIC nanoGUNE and UPV/EHU)

Scientific Committee
Shashank Harivyasi (Graz University of Technology, Graz)
Mato Knez (CIC nanoGUNE, San Sebastian)
Morten Madsen (University of Southern Denmark, Sonderborg)
Moritz Muller (Materials Physics Center, San Sebastian)
Daniel Sánchez-Portal (Materials Physics Center, San Sebastian)
Weike Wang (CIC nanoGUNE, San Sebastian) Organizing Committee

Organizing Committee
Julene Lure (CIC nanoGUNE, San Sebastian)
Itziar Otegui (CIC nanoGUNE, San Sebastian)
Katharina Rubahn Rubhan (University of Southern Denmark, Sønderborg)

The summer school "Surfaces and Interfaces" took place on 20-23 June 2017 in the framework of a European collaborative network of doctorate programs in Physics and Chemistry of Advanced Materials (PCAM), a European initial training network THINFACE, and the Summer Courses of the University of the Basque Country (UPV/EHU). The summer school was held in a seaside palace in the scenic city of San Sebastian, Basque Country (Spain) and welcomed Master and PhD students, post-docs, and all researchers interested in the field. The program, based on tutorials and invited talks, also included oral contributions and posters.

Tutorials
- **Advances in 2D Materials**
  Oliver Monti (University of Arizona, USA)
- **Thin-Film Solar Cells**
  Frank Nüesch (EMPA, Switzerland)
- **Photonics/Plasmonics in 2D Materials**
  Luis Martín-Moreno (Universidad Zaragoza, Spain)
- **Core-level Spectroscopies**
  Franz Himpsel (University of Wisconsin-Madison, USA)

Invited speakers
Stefano Agnoli (Università degli Studi di Padova)
Rainer Hillenbrand (CIC nanoGUNE, Spain)
James O'Shea (University of Nottingham, UK)
Talat Rahman (University of Central Florida, USA)
Koen Vandewal (TU Dresden, Germany)
Karin Zojer (Graz University of Technology, Austria)
Jost Adam (Syddansk University, Denmark)
David Egger (Regensburg University, Germany)
Luca Floreano (Instituto Officina dei Materiali, Italy)

DIPC School

PhotoElectroCatalysis at the Atomic Scale

June 27-30, 2017
Miramar Palace, Donostia / San Sebastián
http://pecas.dipc.org/

Scientific Committee
José Ángel Martín Gago (Instituto de Ciencia de Materiales de Madrid, CSIC)
Doris Grumelli (INIFTA – CONICET)
Miquel Salmerón (Lawrence Berkeley National Lab)
Alexander Weber-Bargioni (Molecular Foundry-Lawrence Berkeley National Lab)
Klaus Kern (Max Planck Institute for Solid State Research)

Organizing Committee
Sara Barja (Ikerbasque, CFM-CSIC-UPV/EHU, DIPC)
Celia Rogero (CFM-CSIC-UPV/EHU, DIPC)
Mato Knez (Ikerbasque, CIC nanogune)
Karmela Alonso (DIPC)

The DIPC School PECAS was aimed at promoting interdisciplinary discussion of scientists in the material science and photoelectrochemistry fields in addition to presentation of new results, ideas and methods to understand the catalyst-electrolyte interface at an atomic level.

The school was taught at the postgraduate level in the fields of surface science and electrochemistry, but introductory seminars were specially addressed to introduce master and graduate students from chemistry and/or physics in each topic covered in the school.

Subjects covered in the school:
• In situ and in operando electrochemistry-surface science techniques and methods
• Energy conversion from photon and chemical energy to electrical energy
• Electrocatalysts for water splitting and CO2 reduction
• Local active sites on solid surfaces: reactivity of defects
• Chemical engineering and synthesis of photoelectrochemical systems
• Novel materials for electrochemical energy storage
• Electrochemical biosensors
• Theoretical modeling of electrochemical interfaces

Invited Speakers
Olaf Magnussen, Christian-Albrechts-Universität zu Kiel
Jan Rossmeisl, University of Copenhagen
Alexander Weber-Bargioni, Molecular Foundry-Lawrence Berkeley National Lab
Craig Banks, Manchester Metropolitan University
José Ángel Martín Gago, Instituto de Ciencia de Materiales de Madrid, CSIC
Doris Grumelli, Instituto de Investigaciones Fisicoquímicas Teóricas y Aplicadas, INIFTA – CONICET
Ulrike Diebold, Technische Universität Wien
Ib Chorkendorff, Technical University of Denmark
Rolf Jürgen Behm, Institute of Surface Chemistry and Catalysis, Ulm University
Ricardo Díez Muiño, Donostia International Physics Center
Alvaro Colina, Universidad de Burgos.
Pau Gorostiza, Institute for Bioengineering of Catalonia

DIPC School

Nanotechnology Meets Quantum Information (NanoQI '17)

July 24-28, 2017
Miramar Palace, Donostia / San Sebastián
http://nanoqi.dipc.org/

Scientific Committee
J.I. Cirac (MPQ Garching)
A. Imamoglu (ETH Zurich)
M.D. Lukin (Harvard University)
G. Giedke (Ikerbasque, DIPC)
Alejandro Gonzalez-Tudela (MPQ Garching)

Advances in nanofabrication and the understanding and control of the quantum properties of matter are laying the groundwork for revolutionary new technologies and information processing capabilities. Following the successful school in 2016, the summer school NanoQI'17 provided an introduction to the basics and recent advances in major areas of quantum information theory and solid-state-based quantum technologies. Both the physics of different implementations of quantum information technologies and the applicable theoretical methods were covered.

The school was aimed at PhD students and young postdocs interested in quantum information processing and quantum technologies. The lectures were given by leading researchers in the field (both from experiment and theory) that offered an overview of the main concepts and methods and explained promising current research directions. In addition there was a forum for all participants to present and discuss their own research with their colleagues and senior researchers.

Eight 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 explore the prospects of quantum computing, quantum technologies, and the physics of quantum many-body systems.

Subjects covered in the school:
• Quantum Information and Quantum Simulations
• Quantum Optics
• Semiconductor Quantum Dots and Spin Qubits
• Circuit-QED and Superconducting Qubits
• Defects in Diamonds for Quantum Information Processing and Metrology
• Quantum Optomechanics
• Solid-state Quantum Optics
• Topological Matter

Invited Speakers
J. Ignacio Cirac (MPQ Garching, Germany)
Rudolf Gross (TU München, Germany)
Fedor Jelezko (U Ulm, Germany)
Atac Imamoglu (ETH Zurich, CH)
Mikhail D. Lukin (Harvard University, USA)
Florian Marquardt (U Erlangen, Germany)
Eugene Polzik (U Copenhagen, Denmark)
Gil Refael (Caltech, Pasadena, USA)
Lieven Vandersypen (TU Delft, Netherlands)
Susanne Yelin (U Connecticut, USA)

DIPC School

Topological Matter School 2017

August 21-25, 2017
Miramar Palace, Donostia / San Sebastián
http://tms17.dipc.org/

Organizing Committee
Reyes Calvo (CIC nanoGUNE)
Dario Bercioux (DIPC)
Maia G. Vergniory (DIPC)
Jérôme Cayssol (LOMA)

This one-week school provided pedagogical lectures by leading experts on the field. The school comprises introductory sessions on group theory and topology supported with practical exercises, including a session on numerical quantum transport calculation of topological systems. There was a number of focus sessions on topological phases of matter such as topological insulators, Weyl semimetals or topological superconductors, including a review session on the major experimental achievements in the field. In addition, a special session was dedicated to the connection between high energy physics and topological matter.

Invited Speakers
Alexander Altland (Cologne)
Jens Bardarson (Dresden/Stockholm)
Haim Beidenkopf (Rehovot)
Andrei Bernevig (Princeton)
Erwann Bocquillon (Paris)
Claudia Felser (Dresden)
Adolfo Grushin (Berkeley/Grenoble)
Titus Neupert (Zurich)
Leslie Schoop (Stuttgart)
Ivo Souza (Donostia / San Sebastián)
Michael Wimmer (Delft)

DIPC Course

Rational Design of 2D Materials

January 2017
DIPC, Donostia / San Sebastián

Prof. Talat S. Rahman
Department of Physics, University of Central Florida, USA and DIPC, Spain

The aim of this course was to lay the foundation for experimental and theoretical work that forms the basis for designing 2D materials with desired functionalities. The approach falls under the umbrella of the Materials Genome Initiative (MGI) in which theory and experiments work in a feedback loop with information from one used to better the other, to accelerate the discovery of novel materials. It was addressed to physics and chemistry students at all stages and senior scientists who are interested in understanding and predicting the characteristics of functional 2D materials. The specific direction and scope of the course was open to discussion and was adjusted to the interest of the audience.

DIPC Course

Introduction to Quantum Many-body Systems and Quantum Information

March 2017
DIPC, Donostia / San Sebastián

J.-Prof. Dr. Roman Orus
Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany

The aim of this course is to provide the basics on the necessary tools to understand quantum many-body systems from a quantum information perspective. We reviewed the theory of quantum entanglement and its quantification, its application in the study of quantum phase transitions, and its implications for quantum matter through the tensor network representation of quantum states. As a practical application, we explained the basics of the Density Matrix Renormalization Group algorithm, the most successful numerical tool in the study of the low-energy properties of 1d quantum lattice systems.

DIPC Course

A Brief Introduction to the Theory of Networks

April 2017
DIPC, Donostia / San Sebastián

Prof. Gabriel Cwilich
Yeshiva University, New York, USA

In this series we covered some basic concepts of networks' theory: their different metrics and measures at the local level and their large structure, and the most common mathematical techniques to study them.

We discussed theoretical models of networks (Poissonian, power-law distributions, configuration models, small-world model) and of network formation (including the Barabasi-Albert model of preferential attachment); and finally some processes in networks (percolation and network resilience and (time permitting) models of spreads of diseases.

DIPC Course

Group Theory in Condensed Matter: A Practical Introduction

September 2017
DIPC, Donostia / San Sebastián

Prof. Juan Luis Mañes Palacios
Facultad de Ciencia y Tecnología, UPV/EHU, Bilbao, Spain

This course gave a practical introduction to the uses of group theory in actual condensed matter problems. The stress was on applications rather than formalism, and the main ideas and techniques in group theory was introduced through practical examples. No previous knowledge of group theory was assumed.

Theses

Nonadiabatic effects in adsorbate-surface interactions from first principles.
Dino Novko
March 2017
Supervisor: Maria Blanco

Ab-initio theoretical study of electronic excitations and optical properties in nanostructures.
Federico Marchesin
July 2017
Supervisor: Daniel Sanchez Portal

Structural and electronic properties of two-dimensional alloys of GdAg2/Ag(111) and GdAu2/Au(111).
Alexander Correa
September 2017
Supervisor: Lucia Vitali

Master's Degree Program

UPV/EHU Research Master's in Nanoscience

DIPC, along with CIC nanoGUNE, 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 Materials Physics Center (CFM-CSIC-UPV/EHU).

The Research Master's in Nanoscience has been offered since 2007 with now close to 120 students having 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.

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