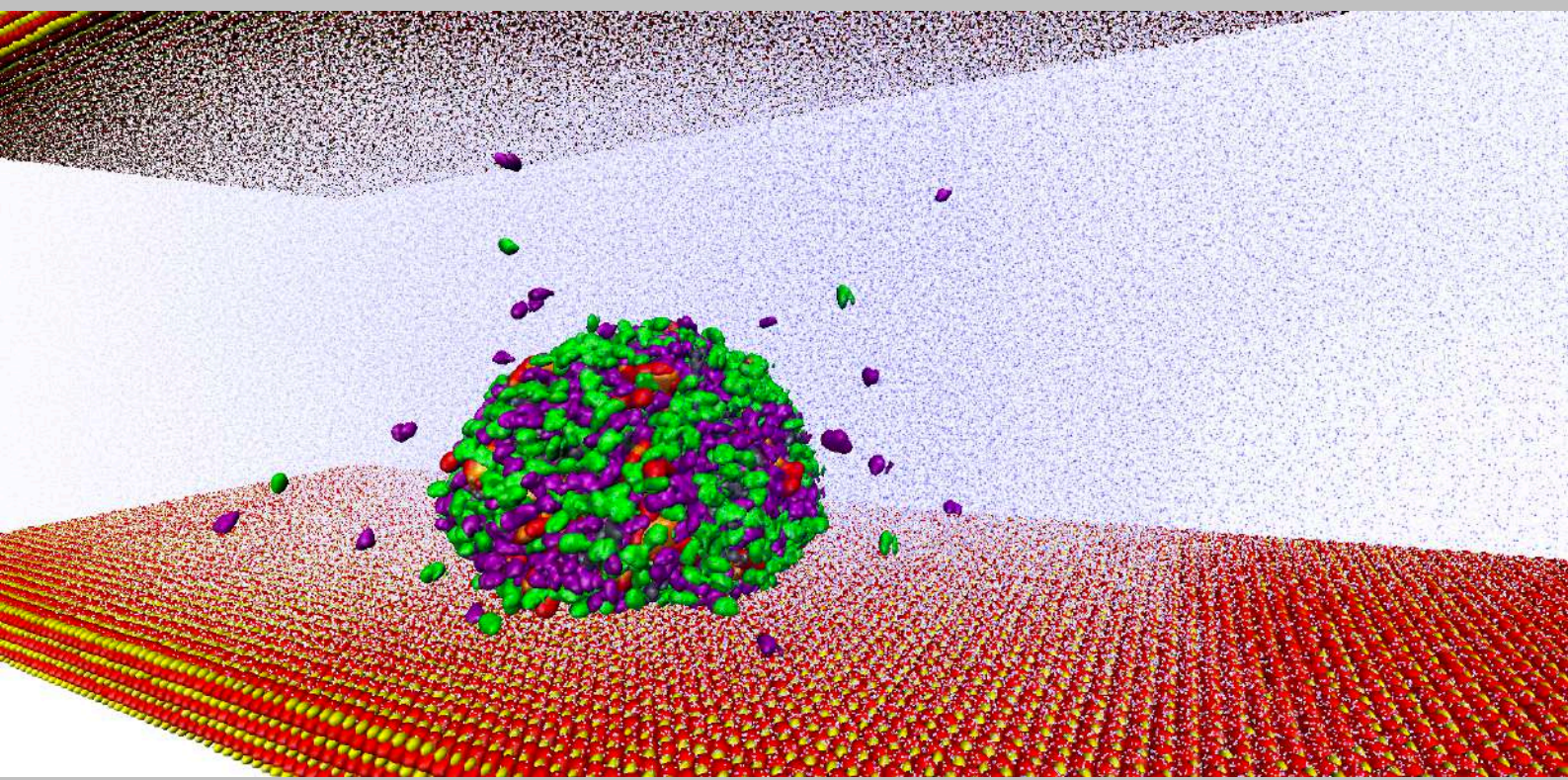
Institut de Química Teòrica
i Computacional
UNIVERSITAT DE BARCELONA

UNIVERSITAT DE BARCELONA

Institut de Química Teòrica i Computacional de la Universitat de Barcelona (IQTCUB)



Activity Report 2016

The creation of the Institute of Theoretical Chemistry of the *Universitat de Barcelona* (IQTCUB) was approved on November 27th, 2007. The IQTCUB members are professors and researchers from different departments of the Chemistry and Physics faculties of UB who employ methods of Computational Chemistry and/or Computational Physics (e.g. Quantum Chemistry, Solid State Modeling). The IQTCUB research activity focuses mainly in the field of Chemistry. Yet, this activity is quite different from what one expects from a traditional chemist. Indeed, the instruments used by the IQTCUB members cannot be found in a typical chemical laboratory but rather in a virtual "computational laboratory" with supercomputers having hundreds or thousands of processors. The main goals of Theoretical and Computational Chemistry are: to achieve a detailed understanding of chemical process at the molecular level, to suggest new experiments by means of predictions that have to be experimentally proven, to interpret and provide a rationale of complex experimental results, and to devise new tools and concepts. Following these general objectives, the IQTCUB aims to design new materials and drug molecules with tailored properties, investigate new chemical reactions to obtain key products with improved efficiency and selectivity, to improve existing processes with respect to efficiency and environmental impact, and to propose new sources of sustainable energy. Although most of these goals are common to other scientific disciplines (given the interdisciplinary approach of modern research), the insights provided by theoretical and computational chemistry are unique and cannot be obtained with other methods. Therefore, the tools developed and employed in IQTCUB play a prime role in solving many pressing challenges faced by modern society.

This has been another difficult year for research budget in Spain and the support from UB through the research deputy has been invaluable. This is fully acknowledged by all personnel of the institute who otherwise could not carry out this research. In fact, without the support from the institution it would be impossible to maintain the computational infrastructure, which is essential to carry out a high-quality and competitive research. This is also thanks to the, often invisible, excellent technical staff that is responsible for keeping the whole computational framework working. This *activity report* evidences the IQTCUB vitality and growth over almost ten years, the considerable scientific production in research lines as diverse as drug design, heterogeneous catalysis, nanostructures, novel materials, and atmospheric chemistry clearly demonstrates the growing impact of our research. We do hope that the IQTCUB project will continue to deserve the support of our university in the years to come. This will certainly be essential to further improve the scientific quality of IQTCUB, which was recently recognized by external peer review evaluation. This year has also been marked by elections for the UB President and we hope that, based on this memoir, the new team will continue with the compromise with the IQTCUB.

Francesc Illas
Director de l'IQTCUB

REPORT CONTENT

I. IQTCUB OVERVIEW

The Institute of Theoretical and Computational Chemistry of the *Universitat de Barcelona* (IQTCUB), was created by the university Government Board on November 27th, 2007, with the main goal of enhancing and supporting scientific research in Theoretical and Computational Chemistry at the *Universitat de Barcelona* by organizing the research in four main lines and promoting and supporting interdisciplinary activities which will allow to tackle the new challenges in this scientific discipline.

I.1 DIRECTION TEAM

Prof. Francesc Illas Riera	*Director*
Prof. Ramón Sayós Ortega	*Treasurer and Secretary*
Prof. Carme Rovira Virgili	*Board member*

I.2 IQTCUB RESEARCH LINES

Scientific research currently being carried out at the IQTCUB can be viewed as classified in the following four main research lines.

1. **Methods, algorithms and computational tools development**

Here we focus on theories and algorithms devoted to account for electronic correlation, nuclear motion, quantum structure-activity, continuous symmetry measures, molecular modelling, variational state transition theory and magnetic resonance. Further developing of Monte Carlo, molecular dynamics and Brownian dynamics is also envisaged.

2. **Computational Materials Science**

In this research area we employ computational methods, ranging from high-level quantum chemistry and ab initio molecular dynamics to classical simulation methods, to investigate the bulk, surface and nanoscale properties of a broad class of solid materials, such as complex inorganic compounds, molecular crystals and heterogeneous catalysts.

3. **Computational Biochemistry and Soft Matter**

Using the arsenal of available computational methods, from electronic structure based methods to classical simulations, we focus on systems of biological interest. In particular we investigate the structure and reactivity of proteins and enzymes, drug design, processes in cellular membranes, enzymatic reactions in crowded media and soft nanoparticles in solution.

4. **Reactivity and Reaction Dynamics**

Research in this area uses quantum, classical and statistical mechanics methods to analyse the dynamics of elementary reactions, electronic excited states and atmospheric and combustion reactions. Continuum methods are also used to investigate macromolecular complexation reactions in aqueous media.

I.3 IQTCUB MEMBERS

IQTCUB involves a total of 96 professors and researchers: The full list of members of IQTCUB (including the corresponding academic situation and affiliation within UB) is provided below.

Family Name	Name	Department/Unit	Section
Full Professors			
Aguilar Navarro	Antonio	Materials Science & Physical Chemistry	Physical Chemistry
Alemany i Cahner	Pere	Materials Science & Physical Chemistry	Physical Chemistry
Alvarez Reverter	Santiago	Inorganic and Organic Chemistry	Inorganic Chemistry
Bofill Villà	Josep Maria	Inorganic and Organic Chemistry	Organic Chemistry
González Pérez	Miguel	Materials Science & Physical Chemistry	Physical Chemistry
Illas Riera	Francesc	Materials Science & Physical Chemistry	Physical Chemistry
Mas Pujadas	Francesc	Materials Science & Physical Chemistry	Physical Chemistry
Novoa Vide	Juan José	Materials Science & Physical Chemistry	Physical Chemistry
Rubio Martínez	Jaime	Materials Science & Physical Chemistry	Physical Chemistry
Ruiz Sabin	Eliseo	Inorganic and Organic Chemistry	Inorganic Chemistry
Sayós Ortega	Ramón	Materials Science & Physical Chemistry	Physical Chemistry
Associate Professors			
Albertí Wirsing	Margarita	Materials Science & Physical Chemistry	Physical Chemistry
Costa Sala	Ramón	Inorganic and Organic Chemistry	Inorganic Chemistry
De Andrés Llopis	Jaime	Materials Science & Physical Chemistry	Physical Chemistry
D. P. Ribeiro Moreira	Ibério	Materials Science & Physical Chemistry	Physical Chemistry
Giménez Font	Xavier	Materials Science & Physical Chemistry	Physical Chemistry
Huarte Larrañaga	Fermín	Materials Science & Physical Chemistry	Physical Chemistry
Lucas Alcorta	Josep Maria	Materials Science & Physical Chemistry	Physical Chemistry
Llunell Marí	Miquel	Materials Science & Physical Chemistry	Physical Chemistry
Mota Valeri	Fernando	Materials Science & Physical Chemistry	Physical Chemistry
Paniagua Valle	Juan Carlos	Materials Science & Physical Chemistry	Physical Chemistry
Solé Sabaté	Albert	Materials Science & Physical Chemistry	Physical Chemistry
Sousa Romero	Carme	Materials Science & Physical Chemistry	Physical Chemistry
Vilaseca Font	Eudald	Materials Science & Physical Chemistry	Physical Chemistry

Other Categories (Professors Agregats)

Aullón López	Gabriel	Inorganic and Organic Chemistry	Inorganic Chemistry
Bonet Ruiz	Jordi	Chem. Engineering & Analytical Chem.	Chem. Engineering
Deumal Solé	Mercè	Materials Science & Physical Chemistry	Physical Chemistry
Díez Pérez	Ismael	Materials Science & Physical Chemistry	Physical Chemistry
Gamallo Belmonte	Pablo	Materials Science & Physical Chemistry	Physical Chemistry
Madurga Díez	Sergio	Materials Science & Physical Chemistry	Physical Chemistry
Ribas Ariño	Jordi	Materials Science & Physical Chemistry	Physical Chemistry
Reigada Sanz	Ramón	Materials Science & Physical Chemistry	Physical Chemistry

Other Categories (Professors Associats)

Figueras Valls	Marc	Materials Science & Physical Chemistry	Physical Chemistry
Jover Modrego	Jesús	Inorganic and Organic Chemistry	Inorganic Chemistry
Roncero Barrero	Cristina	Materials Science & Physical Chemistry	Physical Chemistry
Tercero Mohedano	Javier	Inorganic and Organic Chemistry	Inorganic Chemistry
Valero Montero	Rosendo	Materials Science & Physical Chemistry	Physical Chemistry

ICREA Research Professors

Bromley	Stefan T.	Materials Science & Physical Chemistry	Physical Chemistry
Neyman	Konstantin M.	Materials Science & Physical Chemistry	Physical Chemistry
Poater Teixidor	Jordi	Inorganic and Organic Chemistry	Organic Chemistry
Rovira Virgili	Carme	Inorganic and Organic Chemistry	Organic Chemistry

Postdoctoral contracts

Beatriu de Pinós-Juan de la Cierva

Cirera Fernández	Jordi	Inorganic and Organic Chemistry	Inorganic Chemistry
Echeverría López	Jorge	Inorganic and Organic Chemistry	Inorganic Chemistry
Albareda Piquer	Guillem	IQTCUB	

Marie-Curie

Darwish	Nadim	Materials Science & Physical Chemistry	Physical Chemistry

Ramón y Cajal

Viñes Solana	Francesc	Materials Science & Physical Chemistry	Physical Chemistry

Contracte Projecte de Recerca

Bahamón	Daniel	Materials Science & Physical Chemistry	Physical Chemistry
López Marne	Estefanía	Materials Science & Physical Chemistry	Physical Chemistry
Valero Montero	Rosendo	Materials Science & Physical Chemistry	Physical Chemistry

Other

Alfonso Prieto	Mercedes	Inorganic and Organic Chemistry	Organic Chemistry
Chul Ko	Kyoung	Materials Science & Physical Chemistry	Physical Chemistry
Hjorth Larsen	Ask	Materials Science & Physical Chemistry	Physical Chemistry
Kovács	Gábor	Materials Science & Physical Chemistry	Physical Chemistry
Vilà Casanova	Arnau	Materials Science & Physical Chemistry	Physical Chemistry

Ph.D. Students

CONICYT Grant

Maxwell Villacorta	Lindley	Inorganic and Organic Chemistry	Inorganic Chemistry

FI Grant (Catalan Government Program)

Prats García	Hèctor	Materials Science & Physical Chemistry	Physical Chemistry

FPI Grant (Associated with Spanish Ministry of Science and Education Projects)

Alonso Gil	Santiago	Inorganic and Organic Chemistry	Organic Chemistry
Climent Biescas	Clàudia	Materials Science & Physical Chemistry	Physical Chemistry
Coines López-Nieto	Joan	Inorganic and Organic Chemistry	Organic Chemistry
Falceto Palacín	Andrés	Inorganic and Organic Chemistry	Inorganic Chemistry
Jurado Sáez	Manuel	Materials Science & Physical Chemistry	Physical Chemistry
López Carrasco	Montse	Materials Science & Physical Chemistry	Physical Chemistry
Posada Pérez	Sergio	Materials Science & Physical Chemistry	Physical Chemistry

FPU Grant (Associated with Spanish Ministry of Science and Education)

Alcon Rovira	Isaac	Materials Science & Physical Chemistry	Physical Chemistry
Amoza Dávila	Martín	Inorganic and Organic Chemistry	Inorganic Chemistry
Cortijos Aragones	Albert	Materials Science & Physical Chemistry	Physical Chemistry
Garrido Sagargazu	Eduardo	Materials Science & Physical Chemistry	Physical Chemistry
Mondelo Martell	Manel	Materials Science & Physical Chemistry	Physical Chemistry

ITN UE Grant

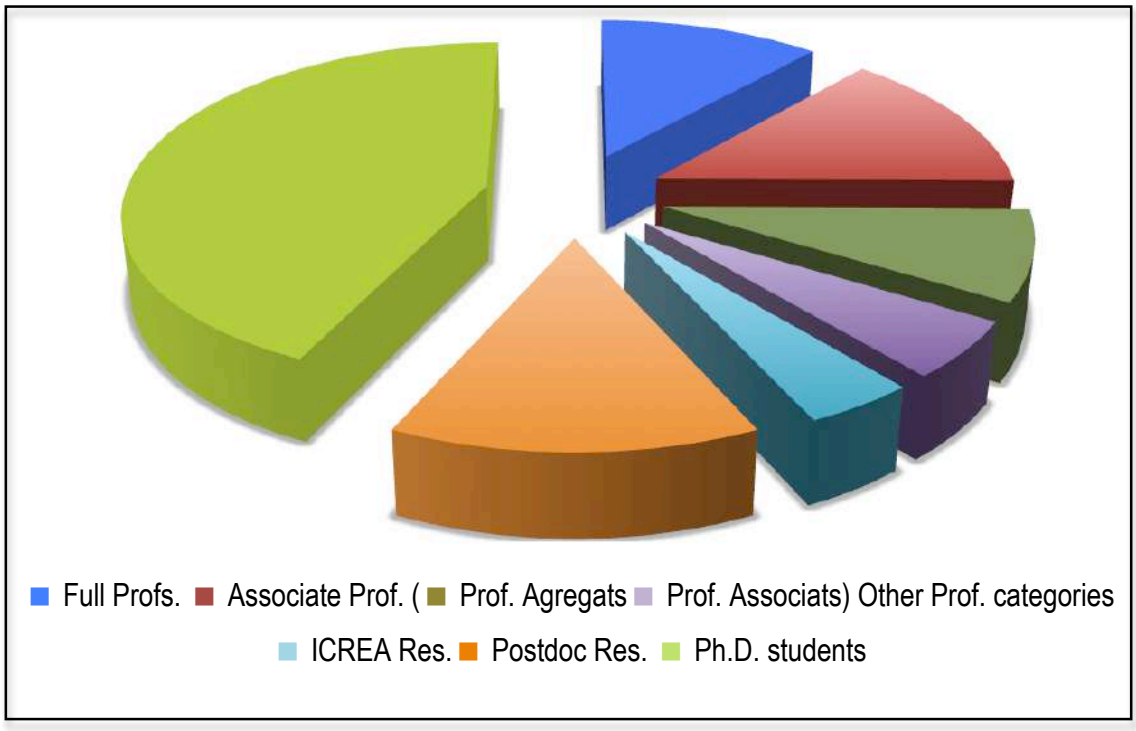
Francese	Tommaso	Materials Science & Physical Chemistry	Physical Chemistry

UB / ADR Grant (University of Barcelona own programme)

Alonso Benito	Gerard	Materials Science & Physical Chemistry	Physical Chemistry
Blancafort Jorquera	Miquel	Materials Science & Physical Chemistry	Physical Chemistry
Lamiel Garcia	J. Oriol	Materials Science & Physical Chemistry	Physical Chemistry
Macià Escatllar	Antoni	Materials Science & Physical Chemistry	Physical Chemistry
Raich Armendáriz	Lluís	Inorganic and Organic Chemistry	Organic Chemistry

Other

Balcells Nadal	Cristina	Materials Science & Physical Chemistry	Physical Chemistry
Bernuz Fitó	Efrem	Inorganic and Organic Chemistry	Organic Chemistry
Blanco Andrés	Pablo Miguel	Materials Science & Physical Chemistry	Physical Chemistry
Cuko	Andi	Materials Science & Physical Chemistry	Physical Chemistry
De Moya	Natalia	Materials Science & Physical Chemistry	Physical Chemistry
Figueroba Sánchez	Alberto	Materials Science & Physical Chemistry	Physical Chemistry
Keshavarz	Sarah	Materials Science & Physical Chemistry	Physical Chemistry
Kunkel	Christian	Materials Science & Physical Chemistry	Physical Chemistry
Manadé Company	Montserrat	Materials Science & Physical Chemistry	Physical Chemistry
Martín Rodríguez	Alejandro	Inorganic and Organic Chemistry	Inorganic Chemistry
Millán Alvares	Maria Angeles	Materials Science & Physical Chemistry	Physical Chemistry
Muñoz Galán	Helena	Materials Science & Physical Chemistry	Physical Chemistry
Nin Hill	Alba	Inorganic and Organic Chemistry	Organic Chemistry
Omidvar	Akbar	Materials Science & Physical Chemistry	Physical Chemistry
Piñero Vargas	Juan José	Materials Science & Physical Chemistry	Physical Chemistry
Pozuelo Ruiz	Marta	Catalan Institute of Bioengineering	
Pueyo Bellafont	Noelia	Materials Science & Physical Chemistry	Physical Chemistry
Reta Mañeru	Daniel	Materials Science & Physical Chemistry	Physical Chemistry
Sopena Moros	Arturo	Materials Science & Physical Chemistry	Physical Chemistry
Vega Domínguez	Lorena	Materials Science & Physical Chemistry	Physical Chemistry
Vilaplana Saiz	Marta	Materials Science & Physical Chemistry	Physical Chemistry



Distribution of IQTCUB members according to the professional category.

I.4 TECHNICAL STAFF

Apart from the academic and research personnel whose main activity is scientific research in theoretical and computational chemistry at IQTCUB, two technical staff members take care of maintenance of the computational infrastructure, their work is extremely important since they also implement the codes and optimize their performance.

Jordi Inglés Camats	*System Administrator Manager*
Teresa Arenal Porcel	*System Administrator*

I.5 EQUIPMENT

Currently, the IQTCUB computational facilities consist of seven calculation clusters located in two conditioned rooms of the Chemistry Faculty of UB. All the clusters except iqtc06 are located in a room near the garage of the faculty where two air conditioning machines of 47,000 and 66.000 KW cool it respectively. Iqtc06 and Iqtc07 are located in a room called VAX, which is cooled by an air conditioner machine of 30.000 KW and another two of 9.000KW.

CALCULATION CLUSTERS

cerqt2 (*invested value 400.000 €*)

Machine type	SUN cluster (4 racks)
Operating system	SLES10
Services	*Calculation cluster and disk server (raid of 2.5TB)*. Internal DHCP server
Structure	Master + 111 nodes
Notes	There are heterogeneous nodes with 32 and 64 bits processors.

Specifications:

Master
CPU: 1.80Ghz Opteron Dual processor (64bits)
RAM: 8GB
HD: 1x146GB hard disk + 2.5TB direct attached storage
Network: 2 gigabit network cards (one for external network and one for calculation network)

7 Sun Fire V60X nodes (3.06Ghz processor)
CPU: 3.06GHz Xeon Dual processor (32 bits)
RAM: 3GB
HD: 2x36GB hard disk
Network: 2 gigabit network cards (calculation network)

92 Sun Fire V60X nodes (2.80GHz processor)
CPU: 2.80GHz Xeon Dual processor (32 bits)
RAM: 6 nodes with 4GB, 86 nodes with 3GB
HD: 2x36GB hard disk
Network: 2 gigabit network cards (calculation network)

11 Sun Fire V20Z nodes (1.80GHz processor)
CPU: 1.80GHz Opteron Dual processor (64 bits)
RAM: 10 nodes with 8GB, 2 nodes with 16GB
HD: 10 nodes with 2x73GB hard disk, 2 nodes with 2x73GB and 2x300GB hard disk respectively
Network: 2 gigabit network cards (calculation network)

1 Sun Fire V20Z node 64 bits (2.20GHz processor)
CPU: 2.20GHz Opteron Dual processor (64 bits)
RAM: 16GB
HD: 2x146GB hard disk
Network: 2 gigabit network cards (calculation network)

iqtc01 (*invested value 250.000 €*)

Machine type	HP cluster
Operating system	Debian Stable
Services	Calculation cluster
Structure	80 nodes
Notes	64 bits processors

Specifications:

80 AMD HP ProLiant DL145 G2 nodes
CPU: 2x2.2GHz AMD Opteron 275 Dualcore
RAM: 8GB
HD: 2x80GB hard disk
Network: 2 gigabit network card (calculation network) + 1 ILO card (out of band network, OOB)

iqtc02 (*invested value 78.000 €*)

Machine type	HP cluster
Operating System	SLES10
Services	Calculation cluster
Structure	26 nodes
Notes	64 bits processors

Specifications:

17 INTEL HP ProLiant DL160 G5 nodes
CPU: 2x2.66GHz Xeon QuadCore
RAM: 16GB
HD: 2x250GB hard disk
Network: 2 gigabit network card (calculation network) + 1 ILO card (OOB)

5 INTEL HP ProLiant DL160 G5 nodes
CPU: 2x2.66GHz Xeon QuadCore
RAM: 16GB
HD: 4x250GB hard disk
Network: 2 gigabit network card (calculation network) + 1 ILO card (OOB)

1 INTEL HP ProLiant DL160 G5 nodes
CPU: 2x2.66GHz Xeon QuadCore
RAM: 16GB
HD: 2x500GB hard disk
Network: 2 gigabit network card (calculation network) + 1 ILO card (OOB)

3 INTEL HP ProLiant DL160 G5 nodes
CPU: 2x2.66GHz Xeon QuadCore
RAM: 32GB
HD: 2x250GB hard disk
Network: 2 gigabit network card (calculation network) + 1 ILO card (OOB)

iqtc03 (*invested value 33.000 €*)

Machine type	HP cluster
Operating System	SLES10
Services	Calculation cluster
Structure	11 nodes
Notes	64 bits processors. Merged with iqtc02 cluster

Specifications:

11 INTEL HP ProLiant DL140 G3 nodes
CPU: 2x2.33GHz Xeon QuadCore
RAM: 16-32GB
HD: 2x80GB hard disk
Network: 2 gigabit network card (calculation network) + 1 ILO card (OOB)

iqtc04 (*invested value 460.000 €*)

Machine type	HP cluster
Operating system	SLES11
Services	Calculation cluster
Structure	101 nodes
Notes	64 bits processors. Infiniband network

Specifications:

95 INTEL HP ProLiant DL160 G6 nodes
CPU: 2x2.66GHz Xeon SixCore
RAM: 48GB
HD: 1x1TB hard disk
Network: 2 gigabit network card (internal data network) + 2 infiniband network (calculation network) + 1 ILO card (IAM)

4 INTEL HP ProLiant DL160 G6 nodes
CPU: 2x2.66GHz Xeon SixCore
RAM: 48GB
HD: 4x500GB hard disk
Network: 2 gigabit network card (internal data network and calculation network) + 1 ILO card (OOB)

2 INTEL HP ProLiant DL160 G6 nodes
CPU: 2x2.66GHz Xeon SixCore
RAM: 48GB
HD: 1x500GB hard disk
Network: 2 gigabit network card (internal data network and calculation network) + 1 ILO card (OOB)

iqtc05 (*invested value 32.000 €*)

Machine type	SGI Cluster
Operating System	SLES11
Services	Calculation cluster
Structure	4 nodes
Notes	64 bits processors

Specifications:

4 AMD SGI H2106-G7 nodes
CPU: 4x2.3GHz Opteron 6276 16-core
RAM: 256GB
HD: 2x1TB hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (OOB)

iqtc06 (*invested value 420.000 €*)

Machine type	Heterogeneous Cluster
Operating System	SLES11
Services	Calculation cluster
Structure	28 nodes
Notes	64 bits processors

Specifications:

25 INTEL HP ProLiant DL560 Gen8 nodes
CPU: 4x2.2GHz Xeon OctoCore
RAM: 512GB
HD: 2x300GB hard disk
Network: 4 gigabit network card (calculation network) + 1 IPMI card (OOB)
Network: 2 10gigabit network card (internal data network)

7 INTEL Supermicro SuperServer 8017R-TF+
CPU: 4x2.3GHz Xeon OctoCore
RAM: 512GB
HD: 3x1TB hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (OOB)
Network: 2 10gigabit network card (internal data network)

iqtc07 (*invested value 40.000 €*)

Machine type	Supermicro Cluster
Operating System	SLES12
Services	Calculation cluster
Structure	2 nodes
Notes	64 bits processors

Specifications:

2 Supermicro 2048U RT4 nodes
CPU: 4x2.6GHZ Intel Broadwell 10Core
RAM: 512GB or 1TB
HD: 1x1TB hard disk
Network: 4 gigabit network card (calculation network) + 1 IPMI card (OOB)
Network: 2 10gigabit network card (internal data network)

GPU cluster (*invested value 47.000 €*)

Machine type	Heterogeneous Cluster
Operating System	SLES11, centos 7
Services	Calculation cluster with GPUs
Structure	*5* nodes
Notes	64 bits processors

Specifications:

Node
CPU: 1x3.06GHz Intel Core i7 950
RAM: 16GB
HD: 1x1TB hard disk
Network: 1 gigabit network card (calculation network)
GPU: 1 NVIDIA GTX580, 1 NVIDIA GTX480

Node Tyan FT72B7015
CPU: 2x2.66GHz Xeon SixCore
RAM: 48GB
HD: 1x500GB hard disk
Network: 4 gigabit network card (calculation network) + 1 IPMI card (OOB)
GPU: 8 NVIDIA GTX580

Node
CPU: 1x3.30GHz AMD FX-4100 QuadCore
RAM: 16GB
HD: 1x1TB hard disk
Network: 1 gigabit network card (calculation network)
GPU: 1 NVIDIA GTX770

Node ASUS ESC4000 G2
CPU: 2x2GHz Xeon SixCore
RAM: 32GB
HD: 1x2TB hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (OOB)
GPU: 4 NVIDIA GTX TITAN

Node ASUS ESC4000 G2
CPU: 2x2.4GHz Xeon SixCore
RAM: 32GB
HD: 1x1TB hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (OOB)
GPU: 4 NVIDIA GTX TITAN BLACK

Node AZServer 4G3S
CPU: 2x2.4GHz Xeon E5-2620v3
RAM: 32GB
HD: 1x1TB hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (OOB)
GPU: 4 NVIDIA GTX 980

Node SIE LADON BROADWELL
CPU: 2x2.4GHz Xeon E5-2640v4 2’4Ghz
RAM: 128GB
HD: 1x1TB hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (OOB)
GPU: 2 NVIDIA TESLA K40

SERVERS

Glusterfs disk server (*invested value 30.000 €*)

Machine type DELL cluster
Operating system SLES 11

Services Storage service cluster with 8TB of space for applications directories and user's work area exported by GlusterFS
Structure 2 nodes
Notes Storage service with a dedicated UPS and redundant power supply

Specifications:

2 INTEL DELL PowerEdge 2950 nodes
CPU: 2x2.50GHz Xeon QuadCore E5420
RAM: 8GB
HD: 4x1TB (raid 5)
Network: 2 gigabit network card (internal network)

Machine type HP cluster
Operating system SLES 11

Services Storage service cluster with 32TB of space for user's data exported by GlusterFS
Structure 2 nodes
Notes Storage service with a dedicated UPS and redundant power supply

Specifications:

1 INTEL HP ProLiant DL180 G6 node
CPU: 2x2.27GHz Xeon QuadCore E5520
RAM: 56GB
HD: 12x2TB (raid 5)
Network: 2 gigabit network card (internal network) + 1 IPMI card (OOB)

1 INTEL HP ProLiant DL380e Gen8 node
CPU: 2x2.20GHz Xeon QuadCore E5-2407
RAM: 48GB
HD: 12x2TB (raid 5)
Network: 2 gigabit network card (internal network) + 1 IPMI card (OOB)

Portal (user access servers) (*invested value 2.300 €*)

Machine type	2 redundant HP ProLiant DL120 G5 nodes
Operating system	Debian stable
Services	SGE Execution Host, Heartbeat, ssh server
Structure	2 redundant nodes
Notes	User access servers for submitting jobs and accessing user data. Critical service connected with a UPS

Specifications:

2 INTEL HP ProLiant DL120 G5 node
CPU: 1x2.33GHz Xeon Dual Core
RAM: 8GB
HD: 1x160GB hard disk
Network: 2 gigabit network card (internal network)

Virtualization servers (*invested value 18.300 €*)

Machine type	4 redundant nodes
Operating system	Debian stable
Services	Xen, DRBD, IQTCUB internal services
Structure	4 redundant nodes
Notes	Servers that contains the Xen virtual machines with the IQTCUB's internal services (SGE, dhcp, license server, etc.). Critical service connected with a UPS

Specifications:

2 INTEL DELL PowerEdge 2950 nodes
CPU: 2x2.50GHz Xeon QuadCore E5420
RAM: 8GB
HD: 2x1TB (raid 1)
Network: 3 gigabit network card (internal network)

2 INTEL HP ProLiant DL120 G5 node
CPU: 1x2.33GHz Xeon Dual Core
RAM: 8GB
HD: 2x160GB hard disk
Network: 3 gigabit network cards (internal network)

Graphical applications server (*invested value 3.000 €*)

Machine type	1 HP ProLiant DL385 node
Operating system	Debian Stable
Services	Server for the use of graphical applications (gaussview, p4vasp, etc.)
Structure	1 node
Notes	Server connected to an UPS

Specifications:

1 AMD HP ProLiant DL385 node
CPU : 2x2.2GHz AMD Opteron 275 Dualcore
RAM: 4GB
HD: 6x146GB hard disk
Network: 1 10/100 network (external network) + 1 gigabit network (internal network)

OTHERS

The IQTCUB have other services to provide service to the IQTCUB's users.

1. Backup server DELL R515 (backup server with 4TB of disk capacity connected to a UPS).
2. Tape library server HP MSL4048 (48 tapes with approximately 48TB of space, ~1TB/tape).
3. Administration server (laptop with 3 network cards for critical incidences support).
4. Proxy server (server that allows the access to the public network from IQTCUB's network).
5. Switch Layer 3 HP Procurve with 24 ports (used for the IQTCUB's date centre infrastructure).
6. 8 Switchs Layer 2 Dlink with 48 ports (internal network for cerqt2, iqtc01, iqtc02, iqtc03 clusters).
7. 4 Switchs Layer 2 HP with 48 ports (internal network for iqtc04, iqtc05 and iqtc06 cluster).
8. 3 Switchs Infiniband Voltaire with 36 ports (calculation network for iqtc04 cluster).

9. Modular switch HP (8 calculation network modules for iqtc01 ,iqtc02, iqtc03 clusters).
10. 2 Modular switch HP 10GB (calculation network for iqtc06 and data network for the glusterfs servers).

The approximated invested cost of this equipment is *50.000 €.*

SUMMARY

Cores ..... 3406 c

Memory ..... 24.736 GB RAM

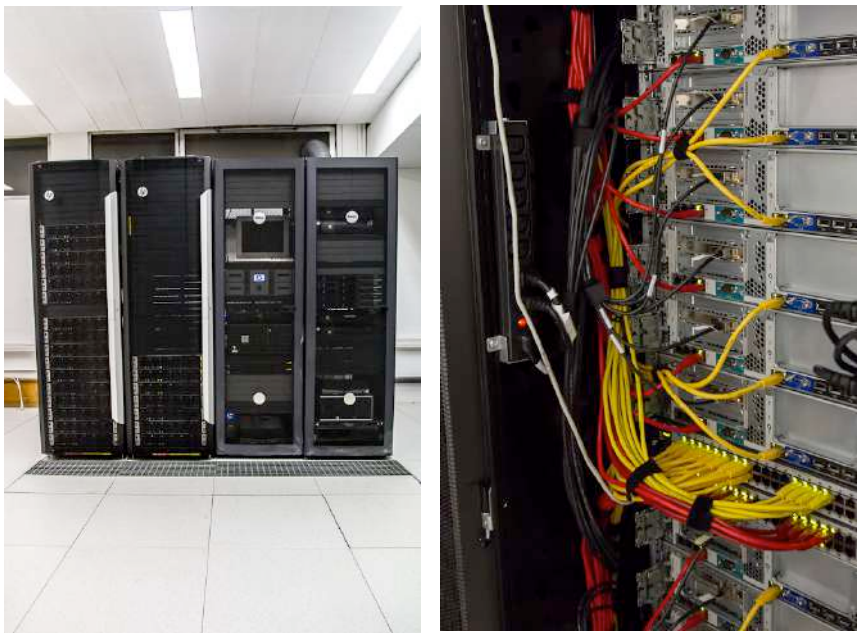
Calculation disk capacity ..... 178 TB

Data user disk capacity ..... 32 TB

The invested amount, considering also the consumables such as network cables and other material is approximately

*1.863.000 €**

*This value does not include the cost of the air conditioning machines and electrical panels.



One of the clusters for intensive calculation in the IQTCUB.

II. IQTCUB ACTIVITIES

II.1 GENERAL ACTIVITIES

Next, a description of activities and actions promoted by IQTCUB through 2016 is provided.

a. ***Promotion and encouragement of research.*** This year the IQTCUB has finally offered three contracts (around 2000 € per contract) aimed to help students to initiate a scientific career. These contracts are addressed to students about to end the degree and aimed to cover a six month period to facilitate the student to pursue an official Master at UB as well as collaborating in some of the research projects of the IQTCUB groups. The contract has been awarded to Lorena Vega Domínguez, Xavier Marugán Ferrer and Enrique Fortín Foz for starting Master studies under the supervision of Drs. Francesc Vinyes, Pere Alemany and Francesc Mas, respectively.

Total cost: 6.246 €

Panel promoting the grants offered for starting research in IQTCUB groups.

b. ***7th IQTCUB workshop.*** This one-day workshop aimed at the dissemination of the research done at the IQTCUB took place on July 10th, 2016 at it was organized by Prof. Mercè Deumal and Dr. Jordi Cirera. The IQTCUB members and internationally acknowledged speakers present the most recent work. This year we highlight the participation of Prof. Walter Thiel from the Max-Planck-Institut für Kohlenforschung with the invited lecture entitled *Surface-hopping excited-state dynamics*, Dr. Jorge Echeverría (*Single molecule motors working on surfaces*), Dr. Rosendo Valero (*Nomad, the novel materials discovery laboratory*), Dr. Gábor Kovács (*Versatile optimization of Chemical ordering in bimetallic nanoparticles*) and Lluís Raich (*Thiolate-protected gold nanoparticles: estructural properties and reactivity*) from the University of Barcelona and IQTCUB, and Dra. Annapaola Migani from the Institut Català de Nanociència i Nanotecnologia (*Theoretical study of heterogeneous photo-catalysis*). Moreover, 19 poster contributions have been presented during the meeting. The IQTCUB assigned a budget to cover the traveling and lodging expenses of Prof. Walter Thiel, the transport expenses of Dra. Annapaola Migani as well as the catering service offered to all assistants.

Total cost: 1.503 €

Panel of the *7th IQTCUB workshop*.

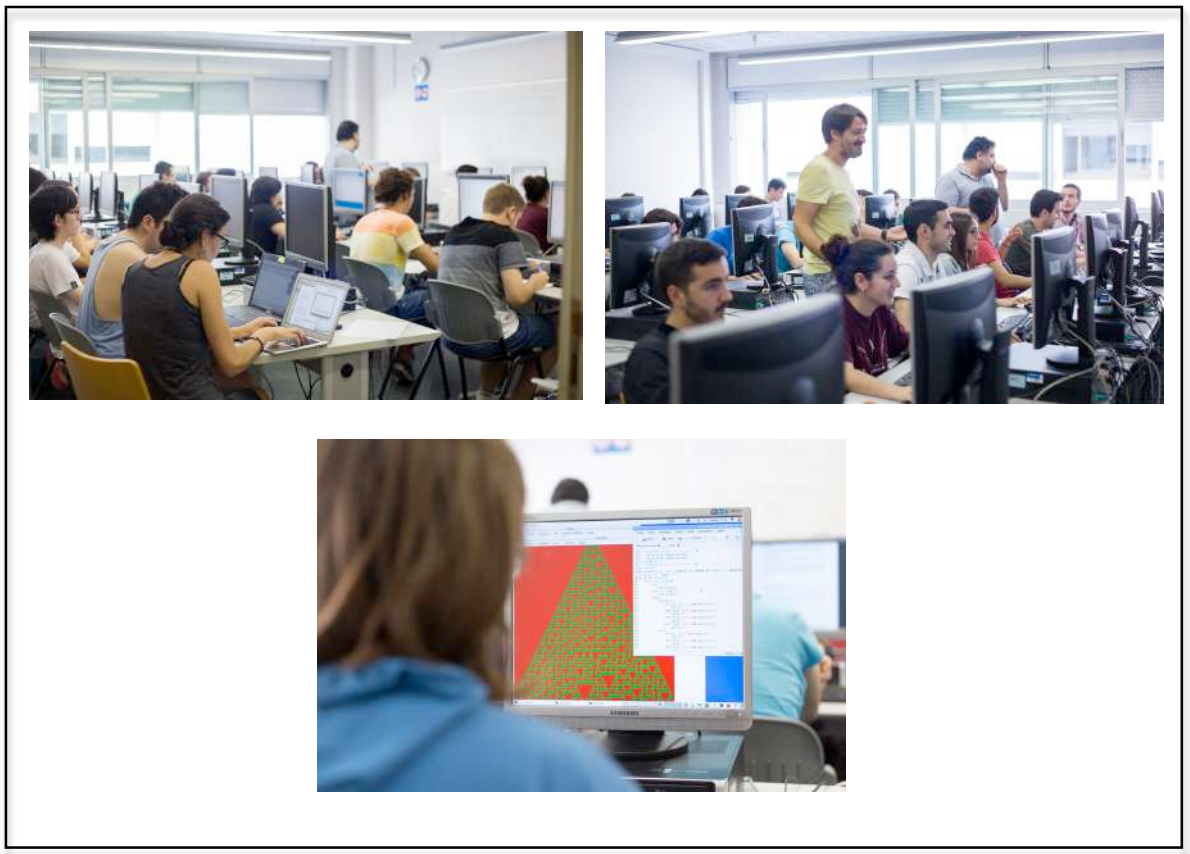
c. ***6th Introductory course in Computational Chemistry.*** The main goal of this course organized by Profs. Fermín Huarte and J. Carlos Paniagua members of the Materials Science and Physical Chemistry Department and the IQTCUB, is to initiate chemistry undergraduate students in the possibilities of Computational Chemistry. The course takes place during a whole week and is mainly addressed to Chemistry and Chemical Engineering students at the University of Barcelona. The 2016 edition has been the sixth one and has been very successful with over 40 students requesting to participate. The different issues exposed along with the teaching staff involved in each session was the following:

1. *Introduction to Linux*, Oriol Lamiel and Gerard Alonso (UB, IQTCUB).
2. *Visualising Biomolecules,* Drs. Carme Rovira and Mercedes Alfonso (UB, IQTCUB).
3. *Structured Programming,* Profs. Albert Solé, Fermín Huarte and J. Carlos Paniagua (UB, IQTCUB).
4. *Cellular Automaton,* Prof. Miquel Llunell and Clàudia Climent (UB, IQTCUB).
5. *Simulation of diffusion by means of Monte Carlo techniques*, Prof. Sergio Madurga (UB, IQTCUB).
6. *Computer Modelling of Materials,* Dr. Stefan Bromley *(UB, IQTC).*
7. *Analysing molecular properties by means of Computational Chemistry Tools,* Prof. Gabriel Aullón (UB, IQTCUB).
8. *Fortran 90,* Prof. Miquel Llunell (UB, IQTCUB).

The present edition took place from June 27th to July 1st, and 24 students performed the registration: V. Advíncula, R. Beato, J. Caldentey, M. Camats, A. Cardenal, R. Cardoso, Z. Fazio, M. Fernández, A. Garcia, P. Lozano, J. Mariñoso, B. Martínez, A. Miró, R. Morales, S. Rafael, M. Ribas, R. Saez, I. Sánchez, R. Terricabres, A. Torres, P. J. Tortajada, S. Trujillo, D. Vázquez and L. Villar.

Total cost: 250 €

Panel of the 6th *Introductory Course in Computational Chemistry* held in 2016.



Some pictures took in this year sessions of the *Introductory Course in Computational Chemistry*.

d. ***5th Advanced Course in Computational Chemistry.*** Fuelled by the positive feedback received from the students in the previous editions we have offered again this year a course at a more advanced level with the main goal of improving previous knowledge in use of computers and, in particular, on Computational Chemistry. Profs. Jaime Rubio and Miguel González from the Materials Science and Physical Chemistry Department of University of Barcelona and IQTCUB have organized the course that has been held in July 4th to 8th. The participants in the course are usually students who have taken part in the Introductory Course or Chemistry undergraduates who have followed a Quantum Chemistry course. In this edition 15 students performed the registration: B. Oró, E. Boldú, M. Camats, B. Martínez, J. Mariñoso, A. Pla, J. Dalmau, M. Garçon, M. Ribas, A. Garcia, C. Privat, J. Bonet, D. Vidal, M. Delgà and J. Sans. IQTCUB has covered breakfast catering expenses of all participants.

Total cost: 240 €

The different issues exposed along with the teaching staff have been the following:

1. *Drug design*, Prof. Jaime Rubio (UB, IQTCUB).
2. *Gas-phase reactions: dynamics and kinetics,* Profs. Miguel Gonzalez and Pablo Gamallo (UB, IQTCUB).
3. *Kinetic Monte Carlo simulations in heterogeneous catalysis*, Prof. Ramon Sayós and Hèctor Prats (UB, IQTCUB).
4. *Enzymatic reactions: QM/MM,* Prof. Rodrigo Martínez Ruiz (Universidad de La Rioja).
5. *Excited states,* Prof. Mercè Deumal (UB, IQTCUB).
6. *Introduction to SGE,* Jordi Inglés and Teresa Arenal *(IQTCUB computing technicians).*
7. *Solid state,* Profs. Iberio Ribeiro and Miquel Llunell (UB, IQTCUB).
8. *Fortran 90,* Prof. Miquel Llunell (UB, IQTCUB).

Panel of the *5th Advanced Course in Computational Chemistry* held in 2016.

Pictures showing the students that shared the *Advanced Course in Computational Chemistry* and their visit to the Mare Nostrum supercomputer (BSC).

e. ***IQTC Internal Seminars*.** In April 2016 started the periodic *IQTC Internal Seminars* in order to disseminate the different research lines of the IQTC groups. The organizers of these seminars are the Ph.D students Isaac Alcón and Manel Mondelo together with Prof. Francesc Illas, all of them members of the IQTC and the Materials Science and Physical Chemistry Department of the University of Barcelona. Here it is the list of the seminars held during 2016:

1. *Towards a first principles description of realistic models of TiO_2 nanoparticles.*
   Oriol Lamiel, april 29, 2016.

2. *Twist is all you need.*
   Isaac Alcón, april 29, 2016.

3. *Catalysts for green chemistry*.
   Sergi Posada, june 17, 2016.

4. *How does the coordination affect the low lying minima in inorganic clusters*.
   Andy Cuko, june 17, 2016.

5. *About a pedagogical approach to DFT.*
   Prof. J. Carlos Paniagua, july 15, 2016.

6. *Time-scale separation of confined and free motions in the H @ SWNT system.*
   Manel Mondelo, october 14, 2016.

7. *Reactivity insights inside the amylosucrase. When occurs the polymerization?*
   Santiago Alonso, october 14, 2016.

8. *On the existence of Pt^{4+} in cerium dioxide: born by nanostructuring.*
   Alberto Figueroba, november 18, 2016.

9. *First-principles theoretical studies on the mechanism of bistability in molecule-based magnets.*
   Tomaso Francese, november 18, 2016.

f. ***Scientific Dissemination Activities.*** Prof. Xavier Giménez Font maintained the online dissemination blog entitled *Chemistry, Air and Environment*, in the magazine *Investigación y Ciencia*. In this blog, it is quite common to find references to the activity and novelties of the research performed by IQTCUB groups. During 2016 the following articles have been published:

1. *From chaos to sustainable energy: carbon dioxide, methane and volcanic lakes.*
   (http://www.investigacionyciencia.es/blogs/fisica-y-quimica/39/posts/del-caos-a-la-energa-sostenible-dixido-de-carbono-metano-y-lagos-volcnicos-14036)

2. *About water magic and some word magicians'.*
   (http://www.investigacionyciencia.es/blogs/fisica-y-quimica/39/posts/acerca-de-la-magia-del-agua-y-de-algunos-magos-de-la-palabra-14098)

3. *Knowledge: teaching almost without master classes: (1) let us accept the challenge.*
   (http://www.investigacionyciencia.es/blogs/fisica-y-quimica/39/posts/acerca-de-la-magia-del-agua-y-de-algunos-magos-de-la-palabra-14098)

4. *Knowledge: teaching almost without master classes: (2) let us do it.*
   (http://www.investigacionyciencia.es/blogs/fisica-y-quimica/39/posts/s-a-b-e-r-ensear-casi-sin-clases-magistrales-ii-hagmoslo-14170)

5. *The ozone is recovering; the global warming is going ahead.*
   (http://www.investigacionyciencia.es/blogs/fisica-y-quimica/39/posts/el-ozono-se-recupera-el-calentamiento-global-contina-14346)

6. *¿Bottled or tap water?*
   (http://www.investigacionyciencia.es/blogs/fisica-y-quimica/39/posts/agua-embotellada-o-agua-del-grifo-14442)

7. *And the light is made: (1) the cosmic grandiosity.* (http://www.investigacionyciencia.es/blogs/fisica-y-quimica/39/posts/y-se-hace-la-luz-i-la-grandiosidad-csmica-14791)

8. *And the light is made: (2) what is fire and other natural subtleties.* (http://www.investigacionyciencia.es/blogs/fisica-y-quimica/39/posts/y-se-hace-la-luz-ii-qu-es-el-fuego-y-otras-sutilezas-naturales-14886)

II.2 IQTCUB SEMINARS AND CONFERENCES

Dr. Stefan Bromley has continued organizing the seminars and conferences of IQTCUB during 2016. A total of ten seminars and/or conferences, which are listed below:

1. **Dr. Martin Goethe** (University of Barcelona) Spain.
   Correcting free energy expressions for thermal motion.
   February 4, 2016.

2. **Dr. Bern Ensing** (Van't Hoff Institute for Molecular Sciences, University of Amsterdam) Netherlands.
   First principle molecular dynamics simulations of electron transfer between aqueous solutes and in photoactive proteins.
   February 16, 2016.

3. **Dr. Jordi Poater** (Organic Chemistry Department, University of Barcelona) Spain.
   B-DNA structure and stability & silylenes stability and reactivity through DFT bonding analyses.
   April 6, 2016.

4. **Prof. Aron Walsh** (University of Bath) UK.
   Solar energy with a twist: dynamic disorder in hybrid perovskites.
   April 22, 2016.

5. **Prof. Célia Fonseca** (Vrije Universiteit Amsterdam) Netherlands.
   The role of aromaticity, hybridization, electrostatics and covalency in resonance-assisted hydrogen bonds.
   April 25, 2016.

6. **Dante Alexander Morales** (Universidad Católica de Santa María de Arequipa) Perú.
   Ciclótidos (Rubiaceae) frente a enfermedades neurodegenerativas.
   July 21, 2016.

7. **Prof. Sergi Garcia-Manyes** (Kings College London) UK.
   Linking mechanochemistry to protein folding at the single bond level.
   November 7, 2016.

8. **Dr. Jocelyne Vreede** (Van't Hoff Institute for Molecular Sciences, University of Amsterdam) Netherlands.
   Path sampling simulations of the mechanisms and rates of transitions between Watson-Crick and Hoogsteen base pairing in DNA.
   November 11, 2016.

9. **Dr. Ivano Tavernelli** (Zürich Research Laboratory) Switzerland.
   TDDFT-based nonadiabatic dynamics with relativistic effects.
   November 17, 2016.

10. **Prof. Nadia Balucani** (University of Perugia) Italy.
    Gas-phase chemistry in extraterrestrial environments.
    December 15, 2016.

II.3 IQTCUB INVITED RESEARCHERS

During 2016, a total of fifteen researchers from all over the world have spent some time at the IQTCUB collaborating in different research projects.

1. **Dr. Angel Morales** (invited visitor).
   Charles University, Czech Republic.
   October 2016.

2. **Prof. Ichraf Oueslati** (COST project visitor).
   University of Paris, France.
   March 2016.

3. **Prof. Ivano Tavernelli** (invited visitor).
   IBM Zürich Research Laboratory, Switzerland.
   November 2016.

4. **Dr. Aaron Kelly** (invited visitor).
   Max Planck Institute for the Structure and Dynamics of Matter, Germany.
   November 2016.

5. **Dra. Noelia Faginas** (invited visitor).
   Università di Perugia, Itàlia.
   September 2016.

6. **Prof. Andrea Lombardi** (invited visitor).
   Università di Perugia, Itàlia.
   September 2016.

7. **Dante Alexander Morales** (invited visitor).
   Universidad Católica de Santa María de Arequipa, Perú.
   July-august 2016.

8. **Diego Ernesto Valencia** (invited visitor).
   Universidad Católica de Santa María de Arequipa, Perú.
   October 2016.

9. **Haruna Luz Barazorda** (invited visitor).
   Universidad Católica de Santa María de Arequipa, Perú.
   October 2016.

10. **Dr. Miroslava Nedyalkova** (Materials networking European project).
    University of Sofia, Bulgaria.
    November 2016.

11. **Prof. Hristiyan Alesandrov** (invited visitor).
    University of Sofia, Bulgaria.
    January-february, july-september 2016.

12. **Prof. Jorge Pavez** (invited visitor).
    Universitat de Santiago de Chile, Chile.
    November 2016.

13. **Prof. Ingrid Ponce** (invited visitor).
    Universitat de Santiago de Chile, Chile.
    September 2016.

14. **Javier Espinoza** (invited visitor).
    Universitat de Santiago de Chile, Chile.
    September 2016.

15. **Prof. Nadia Balucani** (invited visitor).
    University of Perugia, Italy.
    December 2016.

III. SCIENTIFIC ACTIVITY OF IQTCUB MEMBERS

III.1 HIGHLIGHTS FROM MOST RELEVANT RESULTS

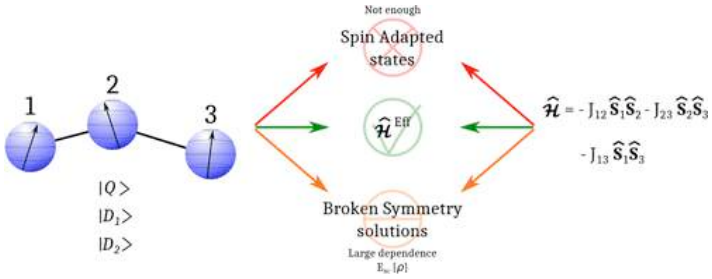
Here some of the most relevant results corresponding to every IQTCUB main research line are presented.

LINE 1. METHODS, ALGORITHMS AND COMPUTATIONAL TOOLS DEVELOPMENT

Magnetic coupling constants in three electrons three centers problems from effective hamiltonian theory and validation of broken symmentry-based approaches

D. Reta, I. de P.R. Moreira, F. Illas.

J. Chem. Theory Comput., *12* (2016) 3228.

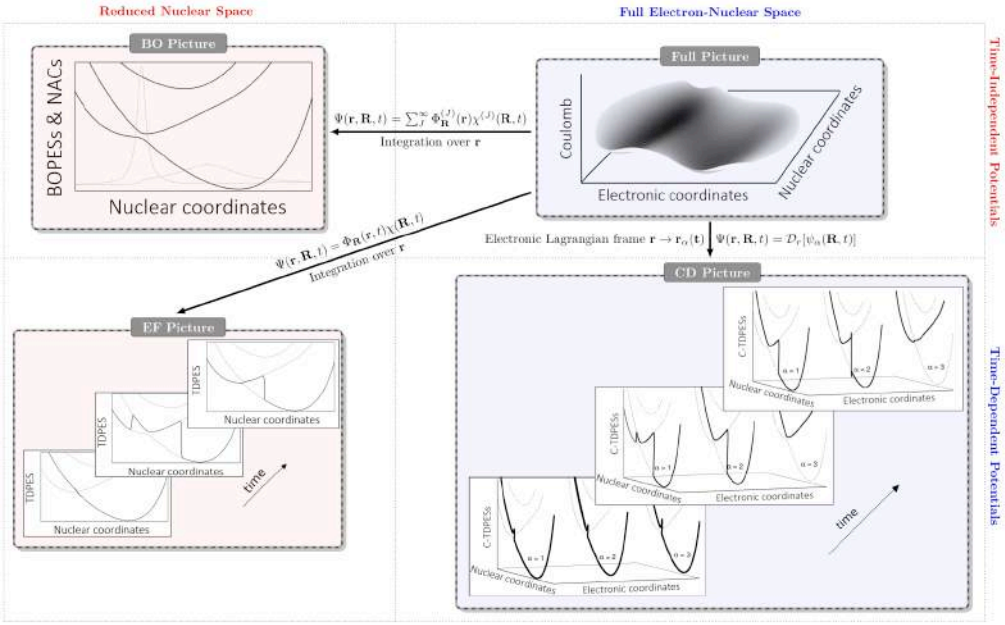


In the most general case of three electrons in three symmetry unrelated centres with S_1 = S_2 = S_3 = ½ localized magnetic moments; the low energy spectrum consists of one quartet (Q) and two doublet (D_1, D_2) pure spin states. The energy splitting between these spin states can be described with the well-known Heisenberg-Dirac-Van Vleck (HDVV) model spin Hamiltonian, and their corresponding energy expressions are expressed in terms of the three different two-body magnetic coupling constants J_{12}, J_{23}, and J_{13}. However, the values of all three magnetic coupling constants cannot be extracted using the calculated energy of the three spin-adapted states since only two linearly independent energy differences between pure spin states exist. In the present work we investigate the 3 electrons in 3 centres problem by means of ab initio effective Hamiltonian theory using MRCI wave functions and validate the broken symmetry approach to extract the J_{12}, J_{23}, and J_{13} in the general non-symmetric case.

Universal steps in quantum dynamics with time-dependent potential-energy surfaces: Beyond the Born-Oppenheimer picture

G. Albareda, A. Abedi, I. Tavernelli, and A. Rubio.

Phys. Rev. A., *94* (2016) 062511.

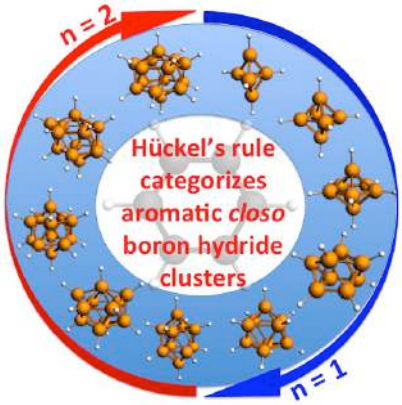


It was recently shown [G. Albareda et al., Phys. Rev. Lett. 113, 083003 (2014)] that within the conditional decomposition approach to the coupled electron-nuclear dynamics, the electron-nuclear wave function can be exactly decomposed into an ensemble of nuclear wave packets effectively governed by nuclear conditional time-dependent potential-energy surfaces (C-TDPESs). Employing a one-dimensional model system, we show that for strong nonadiabatic couplings the nuclear C-TDPESs exhibit steps that bridge piecewise adiabatic Born-Oppenheimer potential-energy surfaces. The nature of these steps is identified as an effect of electron-nuclear correlation. Furthermore, a direct comparison with similar discontinuities recently reported in the context of the exact factorization framework allows us to draw conclusions about the universality of these discontinuities, viz., they are inherent to all nonadiabatic nuclear dynamics approaches based on (exact) time-dependent potential-energy surfaces.

Hückel's rule of aromaticity categorizes aromatic closo boron hydride clusters

J. Poater, M. Solà, C. Viñas, F. Teixidor.

Chem. Eur. J., *22* (2016) 7437.



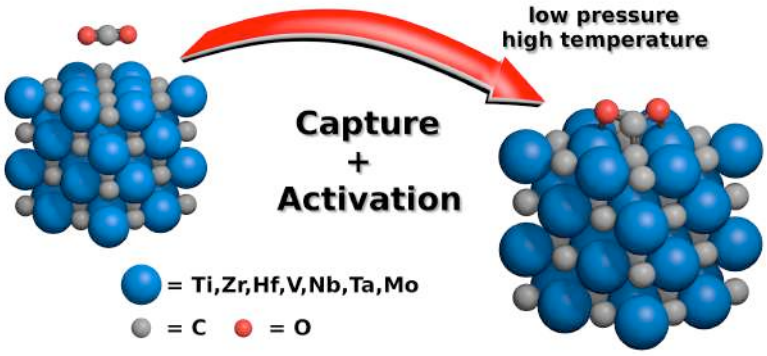
A direct connection is established between three-dimensional aromatic *closo* boron hydride clusters and planar aromatic [*n*]annulenes for medium and large boron clusters. In particular, the results prove the existence of a link between the two-dimensional Hückel rule, as followed by aromatic [*n*]annulenes, and Wade–Mingos' rule of three-dimensional aromaticity, as applied to the aromatic $[B_nH_n]^{2-}$ *closo* boron hydride clusters. The *closo* boron hydride clusters can be categorized into different series, according to the *n* value of the Hückel $(4n+2)\pi$ rule. The distinct categories studied in this work correspond to n = 1, 2, and 3. Each category increases in geometrical difficulty but, more importantly; it is possible to associate each category with the number of pentagonal layers in the structure perpendicular to the main axis. Category 1 has one pentagonal layer, category 2 has two, and category 3 has three.

LINE 2. COMPUTATIONAL MATERIALS SCIENCE

Transition metal carbides as novel materials for CO_2 capture, storage, and activation

C. Kunkel, F. Viñes, F. Illas.

Energy Environ. Sci., *9* (2016) 141.



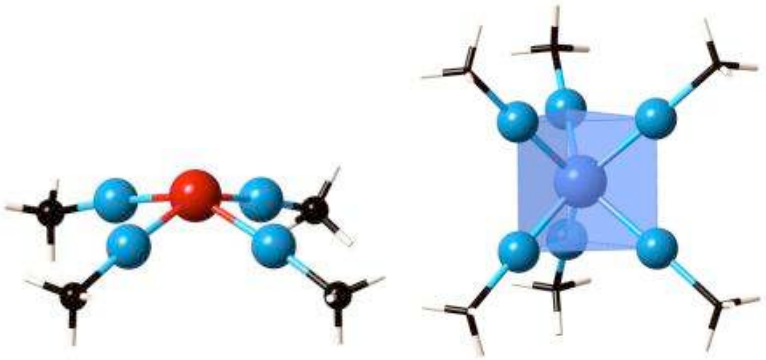
CO_2 is able to adsorb and activate in different transition metal carbides at low pressures and even high temperatures.

The capture and activation of the greenhouse gas carbon dioxide (CO_2) is a prerequisite to its catalytic reforming or breakdown. Here we report, by means of density functional theory calculations including dispersive forces, that transition metal carbides (TMC; TM = Ti, Zr, Hf, Nb, Ta, Mo) are able to uptake and activate CO_2 on their most-stable (001) surfaces with considerable adsorption strength. Estimations of adsorption and desorption rates predict a capture of CO_2 at ambient temperature and even low partial pressures, suggesting TMCs as potential materials for CO_2 abatement.

From widely accepted concepts in coordination chemistry to inverted ligand fields

R. Hoffmann, S. Alvarez, C. Mealli, A. Falceto, T. J. Cahill, T. Zeng, G. Manca.

Chem. Rev., *116* (2016) 8173.



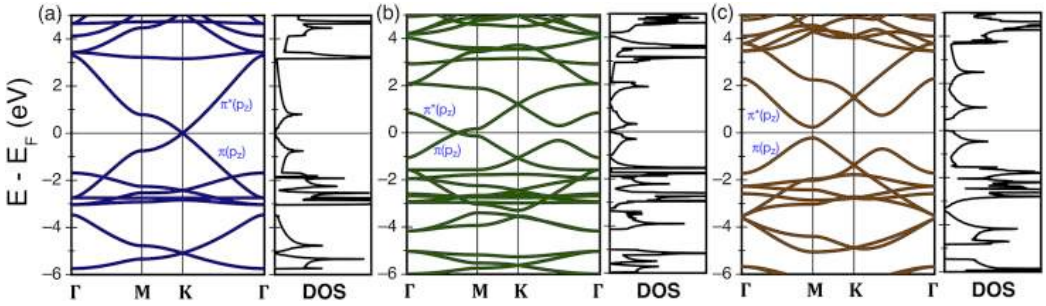
Proposed complexes with inverted ligand fields: $[Rh(AlMe)_4]^+$ i $[Mo(AlMe)_6]$.

We have designed a strategy for inverting the normal splitting of the metal d orbitals in the presence of a ligand field and computationally constructed several examples with a hypothetical but not unrealistic $AlCH_3$ ligand. Special attention is paid to the square-planar case, exemplified by $[Cu(CF_3)_4]^-$, in which Snyder had the foresight to see a case of an inverted field, with the empty valence orbital being primarily ligand centered, the d_{x2-y2} orbital heavily occupied, in what would normally be called a Cu(III) complex. For $[Cu(CF_3)_4]^-$ we provide theoretical evidence from electron distributions, geometry of the ligands, thermochemistry of molecule formation, and the energetics of abstraction of a CF_3 ligand by a base, all consistent with oxidation of the ligands in this molecule. Exploration of inverted ligand fields helps us see the continuous, borderless transition from transition metal to main group bonding. We also give voice to a friendly disagreement on oxidation states in these remarkable molecules.

First-principles study of structural, elastic and electronic properties of α-, β- and γ-graphyne

A. Ruiz-Puigdollers, P. Gamallo.

Carbon *96* (2016) 879.



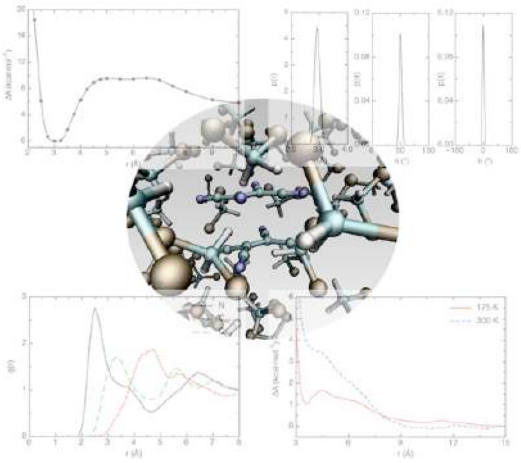
Band structure and total density of states for (a) α-. (b) β-, and (c) γ-graphyne.

This study presents different properties of 2D carbon allotropes: α-, β- and γ-graphynes based on Density Functional Theory calculations. Among the set of properties studied there are structural (*e.g.,* cohesive energies, optimum lattice parameters, interatomic distances, pore sizes, planar packing densities and specific surface areas), mechanical (*e.g.,* uniaxial along with homogeneous and heterogeneous biaxial strains, in-plane stiffness and Poisson's ratio) and electronic properties (*e.g.,* band structures, total and projected density of states, Dirac points or band gap location, Fermi velocity associated to the formers and the effective masses of the carriers associated to the latter). Basically, graphynes present lower values than graphene for cohesive energy, planar packing density, in-plane stiffness and Fermi velocities. Contrarily, graphynes posses a higher variety of pore sizes and a higher Poisson's ratio. These facts make graphynes potential candidates for a wide variety of membrane separations and for applications that need softer materials but maintaining, in a lower extent, some of the electronic properties considered exceptional in graphene.

Formation of long, multicenter π-$[TCNE]_2^{2-}$ dimers in solution: solvation and stability assessed through molecular dynamics simulations

M. Capdevila-Cortada, J. Ribas-Ariño, A. Chaumont, G. Wipff, J. J. Novoa.

Chem. Eur. J., 22 (2016) 17037.

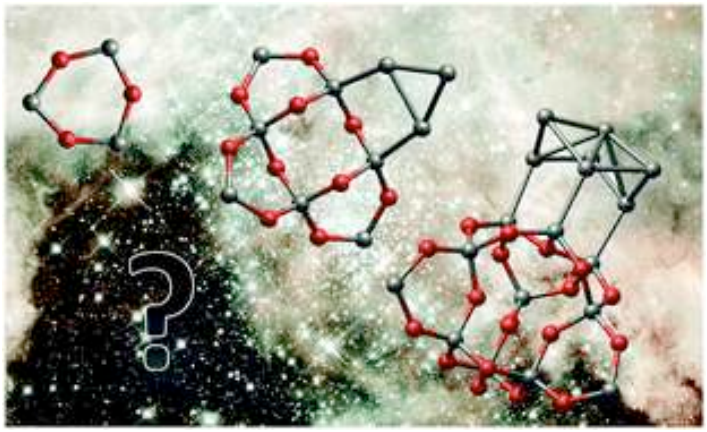


Organic radical-ions dimerize in solution at low temperature forming long, multicenter bonds, despite the metastability of the isolated dimers. In this article, we presented the first computational study of these π-dimers in solution, with explicit consideration of solvent molecules and finite temperature effects. By means of force-field and *ab initio* molecular dynamics and free energy simulations, the structure and stability of π-$[TCNE]_2^{2-}$ dimers in dichloromethane was evaluated. While dimers dissociate at room temperature, they are stable at 175 K and their structure is similar to the one in the solid-state, with a cofacial arrangement of the radicals at an interplanar separation of ca. 3.0 Å. The π-$[TCNE]_2^{2-}$ dimers form dissociated ion pairs with the NBu_4^+ counterions, and their first solvation shell comprises ca. 20 CH_2Cl_2 molecules. Among them, the 8 molecules distributed along the equatorial plane of the dimer play a key role in stabilizing the dimer via bridging C-H···N contacts. The calculated free energy of dimerization of $TCNE^{\cdot-}$ in solution at 175 K is 5.5 kcal mol^{-1}. These results provide the first quantitative model describing the pairing of radical-ions in solution, and demonstrate the key role of solvation forces on the dimerization process.

Under what conditions does $(SiO)_N$ nucleation occur? A bottom-up kinetic modelling evaluation

S. T. Bromley, J. C. Gómez Martín, J. M. C. Plane.

Phys. Chem. Chem. Phys., *18* (2016) 26913.

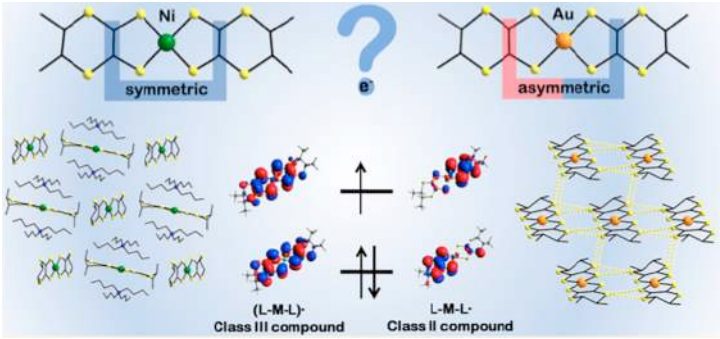


Although nano-sized and nano-segregated SiO has great technological potential and is of enormous astronomical interest, an accurate general description of SiO nucleation is lacking. We provide a state-of-the art evaluation of the range of pressure and temperature conditions for which formation of SiO will or will not proceed.

Localization versus delocalization in chiral single component conductors of gold bis(dithiolene) complexes

D.G. Branzea, F. Pop, P. Auban-Senzier, R. Clerac, P.Alemany, E. Canadell, N. Avarvari.

J. Am. Chem. Soc., *138* (2016) 6838.



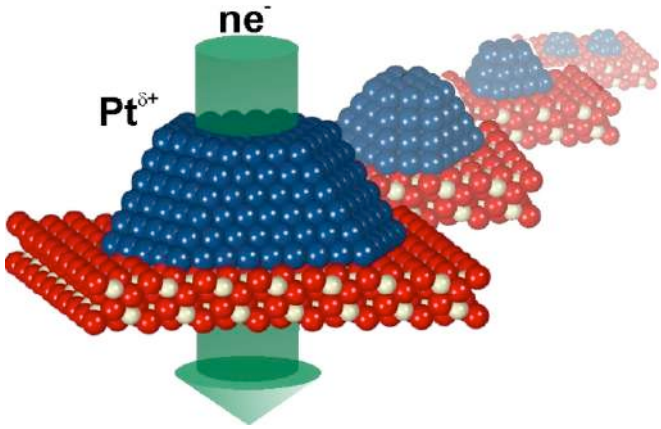
Neutral [Au(dm-dddt)$_2$] complexes have an asymmetric structure and a mixed-valence nature with important consequences in its electrical conductivity in the solid state.

In this work we report the first examples of chiral single component conductors. Both (S,S) and (R,R) enantiomers of the 5,6-dimethyl-5,6-dihydro-1,4-dithiin-2,3-dithiolate (dm-dddt) ligand have been used to prepare neutral [M(dm-dddt)$_2$] (M = Au, Ni) complexes. The most peculiar structural feature concerns a dissymmetry between the two dithiolene moieties for the Au compound, while the Ni counterpart is symmetric. Resistivity measurements show thermally activated behaviour for the open-shell gold complexes, with activation energies strongly influenced by hydrostatic pressure. A thorough theoretical study on Ni anion radical and Au neutral radical bis(dithiolene) complexes addressing the issue of symmetry versus asymmetry from an electronic coupling perspective between the two dithiolene ligands is presented. It results that neutral Au complexes with dithiolene ligands without extended delocalization are Class II mixed-valent compounds in the Robin and Day classification, presenting an inherent tendency toward asymmetric structures, which can be however modulated by the intermolecular organization in the solid state.

Counting electrons on supported nanoparticles

Y. Lykhach, S. M. Kozlov, T. Skála, A. Tovt, V. Stetsovych, N. Tsud, F. Dvořák, V. Johánek, A. Neitzel, J. Mysliveček, S. Fabris, V. Matolín, K. M. Neyman, J. Libuda.

Nature Materials *15* (2016) 284.



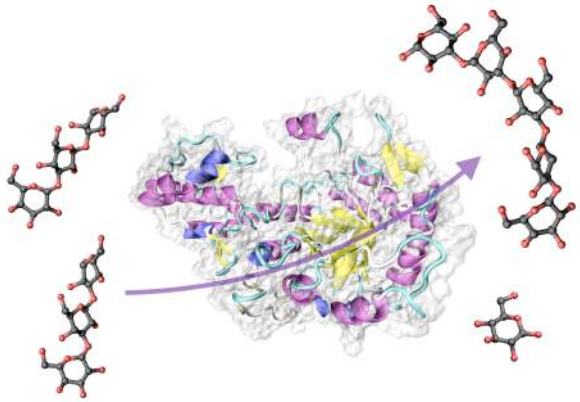
Electronic interactions between metal nanoparticles and supports are the key to advanced catalytic materials. By combining model experiments and theory, we answer a long-standing question related to such interactions: What is the charge on a supported catalyst particle? We quantify the charge transfer for the practically important case of ceria-supported platinum particles and rationalize the origin of its size dependence.

LINE 3. COMPUTATIONAL BIOCHEMISTRY AND *SOFT MATTER*

A trapped covalent intermediate of a glycoside hydrolase on the pathway to transglycosylation. Insights from experiments and QM/MM simulations

L. Raich, V. Borodkin, W. Fang, J. Castro-López, D. van Aalten, R. Hurtado-Guerrero, C. Rovira.

J. Am. Chem. Soc., *138* (2016) 3325.



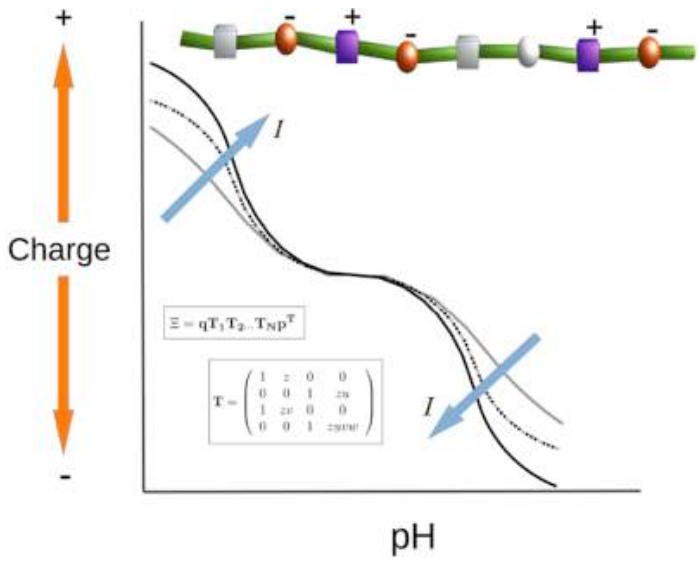
Enzymatic reaction catalyzed by tranglycosylases (synthesis of a glycosidic bond).

The conversion of glycoside hydrolases into transglycosylases, *i.e.* from enzymes that hydrolyze carbohydrates to enzymes that synthesize them, represents a promising solution for the large scale synthesis of complex carbohydrates for biotechnological purposes. However, the lack of three-dimensional enzyme structures and the limited knowledge of the enzyme molecular mechanism at atomic level hampers the rational design of these enzymes. Here we present the first crystallographic structure of a reaction intermediate of a transglycosylase enzyme in complex with an intact carbohydrate. By means of computer simulations, we demonstrate that the enzyme is tuned to catalyze the formation of a new glycosidic bond (transglycosylation reaction) and propose that the variation of a given amino acid would improve significantly the synthetic activity of this family of enzymes.

Dealing with long-range interactions in the determination of polyelectrolyte ionization properties. Extension of the transfer matrix formalism to the full range of ionic strengths

J. L. Garcés, S. Madurga, C. Rey-Castro, F. Mas.

J. Polym. Sci. Part B. Polym. Phys., *doi: 10.1002/polb.24269*.

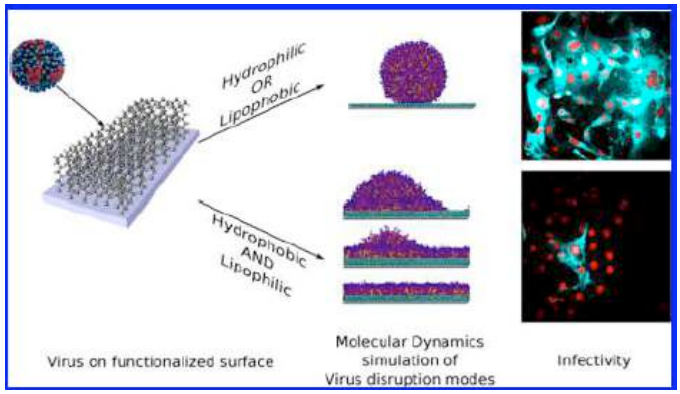


The transfer matrix technique is a very powerful technique to solve Ising-type models of proton binding to polyelectrolytes, but its use is restricted to short range interactions. This work extends the technique to include long range interactions. The resulting titration curves that correspond to different binding models (homogeneous, heterogeneous, polyampholytes) are extremely accurate and indistinguishable in practice from those obtained by Monte Carlo simulations.

Functionalized surfaces with tailored wettability determine influenza A infectivity

I. Mannelli, R. Reigada, I. Suárez, D. Janner, A. Carrilero, P. Mazumder, F. Sagués, V. Pruneri, M. Lakadamyali.

ACS Applied Materials and Interfaces, *8* (2016) 15058.



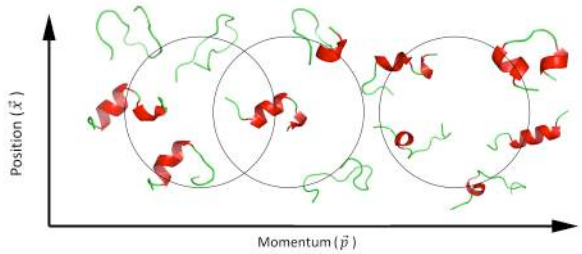
The contact of a virus on a functionalized surface leads to a variety of interaction modes and eventually to the disruption of its lipidic envelope reducing the virus infectivity.

Surfaces contaminated with pathogenic microorganisms contribute to their transmission and spreading. The development of “active surfaces” that can reduce or eliminate this contamination necessitates a detailed understanding of the molecular mechanisms of interactions between the surfaces and the microorganisms. We studied the effects of surfaces functionalized with alkyl- and fluoro-silanes on the infectivity of Influenza A viruses using a number of experimental and computational methods including real-time fluorescence microscopy and molecular dynamics simulations. We show that surfaces that are simultaneously hydrophobic and oleophilic are more efficient in deactivating enveloped viruses. Our results suggest that the deactivation mechanism likely involves disruption of the viral membrane upon its contact with the alkyl chains. These combined features make these substrates highly promising for applications in hospitals and similar infrastructures where antiviral surfaces can be crucial.

Assessment of the sampling performance of multiple-copy dynamics versus a unique trajectory

J. J. Pérez, M. S. Tomas, J. Rubio-Martínez.

J. Chem. Inf. Model., *56* (2016) 1950.



Mostreig de l'espai configuracional amb múltiples trajectòries

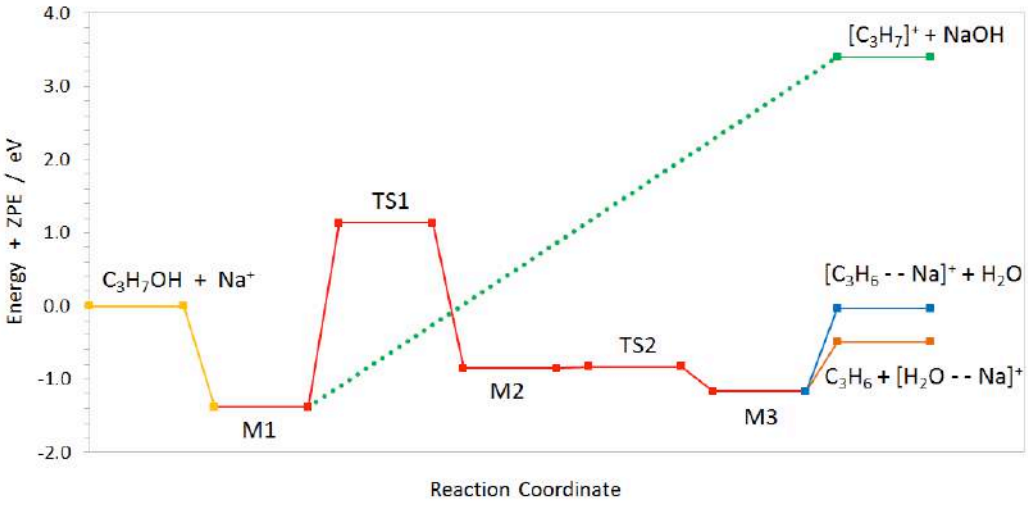
In this work we did an extensive study to ascertain the differential performance of a long molecular dynamics trajectory versus several shorter ones starting from different points in the phase space and covering the same sampling time. For this purpose we selected the $Bak_{16}BH3$ peptide as model of study and carried out several samplings in explicit solvent. Samplings include a 8 μs trajectory; two 4 μs; four 2 μs; eight 1 μs; sixteen 0.5 μs and eighty 0.1 μs. Moreover, the 8 μs trajectory was further extended to 16 μs to have reference values of the diverse properties measured. As a conclusion our results suggest that a few short MD trajectories might provide a better sampling than one unique trajectory. However, caution should be exercised since short trajectories need to be long enough to overcome local barriers surrounding the starting point. An effective way to get insight into the minimum MD trajectory length requires monitoring the convergence of a structural feature, as for example the helical content of the peptide.

LINE 4. REACTIVITY AND REACTIONS DYNAMICS

Dehydrohalogenation and dehydration reactions of *i*-C_3H_7Br and *i*-C_3H_7OH by sodium Ions studied by guided ion beams techniques and quantum chemical methods

E. López, J. M. Lucas, J. De Andrés, M. Albertí, J. M. Bofill, A. Aguilar.

J. Phys. Chem. A, *120* (2016) 4758.



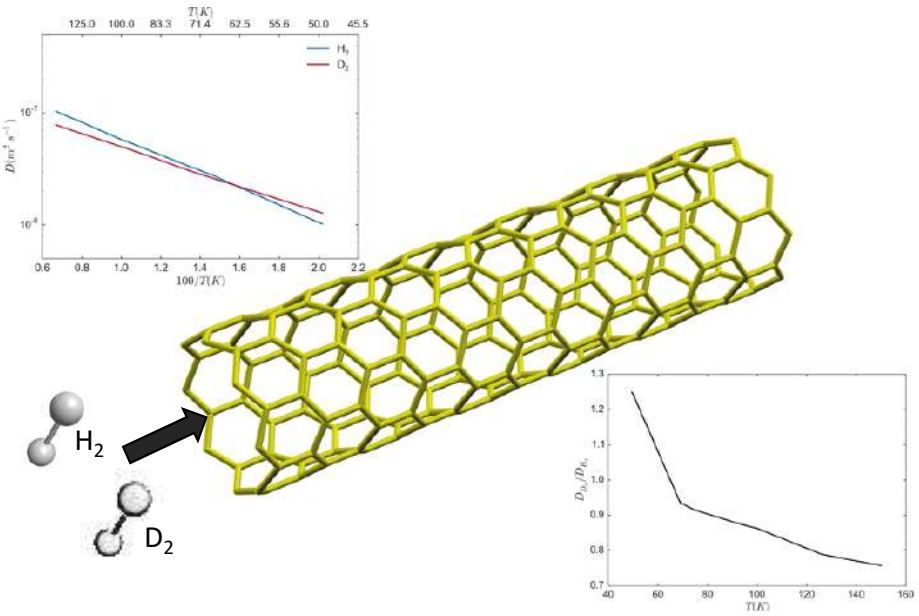
Schematic ZPE profile along the reaction path calculated at the *ab initio* MP2 level on the singlet ground state of the Na^+ + *i*-C_3H_7OH collision system showing the different minima (M) and transition states (TS1) on the PES and their IRC connectivity.

Elimination reactions of gas phase *i*-C_3H_7Br and *i*-C_3H_7OH induced by collision with Na^+ in their electronic ground state were studied experimentally in a radiofrequency-guided ion beam (RF-GIB) apparatus and covering the 0.10 - 10.00 eV center of mass energy range. Na^+ + *i*-C_3H_7Br leads to form $[Na–i\text{-}C_3H_7Br]^+$, $[C_3H_6–Na]^+$, $[HBr–Na]^+$ and $C_3H_7^+$ while for Na^+ + *i*-C_3H_7OH only $[Na–i\text{-}C_3H_7OH]^+$, $[H_2O–Na]^+$ and $C_3H_7^+$ were found. For all products absolute excitation functions were measured and from them rate constants for the formation of $[C_3H_6–Na]^+$, $[HBr–Na]^+$ and $[H_2O–Na]^+$ at 303 K were obtained. *Ab initio* structure calculations at the MP2 level gave information on potential energy surfaces/PES) where elimination and decomposition reactions evolve adiabatically, characterizing different minima and transition state connected along the IRC. PES topology features allow a qualitative interpretation of the experimental data and show the role of the sodium ion as a catalyst in elimination reactions.

Diffusion of H_2 and D_2 confined in single-walled carbon nanotubes: quantum dynamics and confinement effects

M. Mondelo-Martell, F. Huarte-Larrañaga.

J. Phys. Chem. A *120* (2016) 6501.



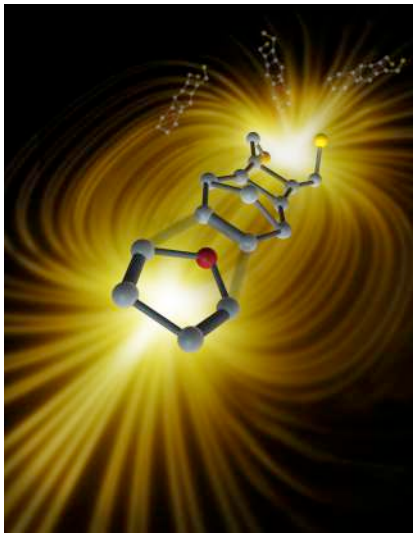
Center figure is an illustration of the diffusion process of H_2 and D_2 in a SWCNT. Top figure plots de computed diffusion constants as a function of 100/T. The bottom figure represents the selectivity coefficient as a function of temperature.

In this publication we present quantum dynamics calculations of the diffusion constant of H_2 and D_2 along a single-walled carbon nanotube at temperatures between 50 and 150 K. We calculate the respective diffusion rates in the low pressure limit by adapting the flux correlation function formalism from the chemical dynamics field to the hopping model used in diffusion simulations. Two different Potential Energy Surfaces are employed to model the C-H interaction. Our results predict a usual kinetic isotope effect, with H_2 diffusing faster than D_2 in the higher temperature range, but a reverse trend at temperatures below 50-70 K. These findings are consistent with experimental observation in similar systems, and can be explained by the different effective size of both isotopes resulting from their different Zero Point Energy.

Electrostatic catalysis of a Diels-Alder reaction

A. C. Aragonès, N. L. Haworth, N. Darwish, S. Ciampi, N. J. Bloomfield, G. G. Wallace, I. Diez-Perez, M. L. Coote.

Nature, *531* (2016) 88.

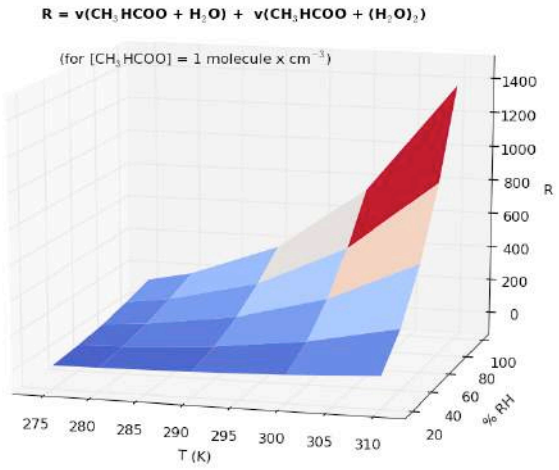


The publication represents the first experimental demonstration of catalysis of a C-C formation reaction with non-redox reagents under the effect of an oriented external electrostatic field. The results open new challenges in the design of synthetic industrial chemical processes using an electric field as a catalyst for the reaction.

Impact of the water dimer on the atmospheric reactivity of carbonyl oxides

J.M. Anglada, A. Solé.

Phys. Chem. Chem. Phys., *18* (2016) 17698.

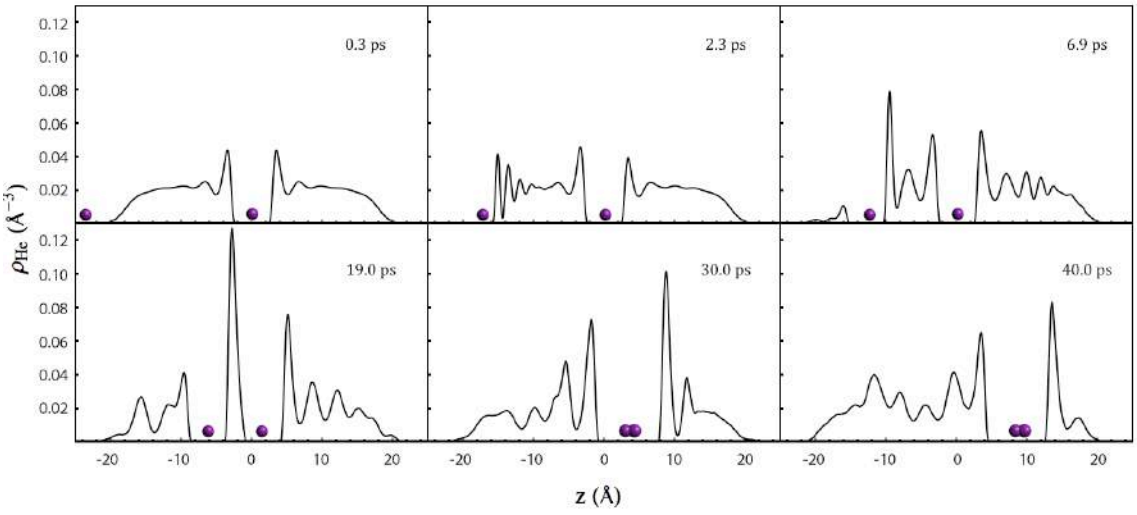


The reactions of twelve carbonyl oxides or Criegee intermediates with the water monomer and with the water dimer have been investigated employing high level theoretical methods. The study includes all possible carbonyl oxides arising from the isoprene ozonolysis and the methyl and dimethyl carbonyl oxides that originated from the reaction of ozone with several hydrocarbons. These reactions have great significance in the chemistry of the atmosphere because Criegee intermediates have recently been identified as important oxidants in the troposphere and as precursors of secondary organic aerosols. Moreover, water vapour is one of the most abundant trace gases in the atmosphere and the water dimer can trigger the atmospheric decomposition of Criegee intermediates. Our calculations show that the nature and position of the substituents in carbonyl oxides play a very important role in the reactivity of these species with both the water monomer and the water dimer. This fact results in differences in rate constants of up to six orders of magnitude depending on the carbonyl oxide. In this work we have defined an effective rate constant (k_{eff}) for the atmospheric reaction of carbonyl oxides with water vapour, which depends on the temperature and on the relative humidity as well. With this k_{eff} we show that the water dimer, despite its low tropospheric concentration, enhances the atmospheric reactivity of Criegee intermediates, but its effect changes with the nature of carbonyl oxide, ranging between 59 and 295 times in the most favourable case (syn-methyl carbonyl oxide), and between 1.4 and 3 times only in the most unfavourable case.

Reaction dynamics inside superfluid helium nanodroplets: the formation of the Ne_2 molecule from Ne + Ne@(^4He)$_N$

A. Vilà, M. González.

Phys. Chem. Chem. Phys., *18* (2016) 31869.



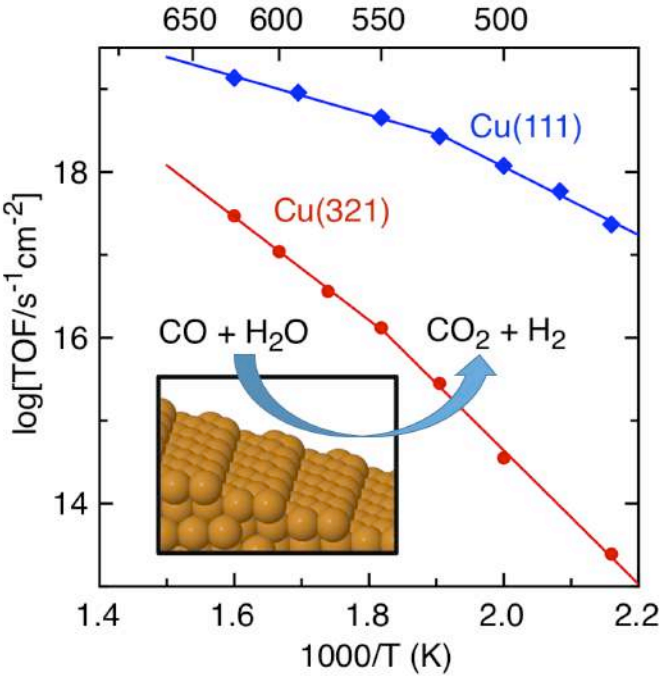
Snapshots showing the time evolution of the helium density along the Ne-Ne axis (z axis) for the Ne + Ne@(^4He)$_{500}$ reaction at the initial average velocity of Ne of 300 m/s (J=0).

The hybrid TDDFT approach proposed by us (J. Chem. Theory Comput., 2015, 11, 899) was extended to reactive processes involving a superfluid helium nanodroplet [A + B@$^4He_{Nv}$ AB@$^4He_{N'}$ + (N-N')^{4}He]; T=0.37 K. This is the first theoretical attempt to study the reaction dynamics of bimolecular type processes involving ^4He_N and the Ne + Ne@^4He_N reaction was considered as the first application example (J=0). We examined the influence of the nanodroplet size (N=200-1000) and initial velocity of the outer Ne atom (<v_0>=120-1000 m/s). The inner Ne atom only produces a greater reduction of the velocity of the outer Ne atom in comparison to what happens in the case of the capture of a Ne atom by a pure nanodroplet. The formation of the molecule is a complex phenomenon related with the nature of the helium density waves produced and their reflection from the nanodroplet surface. This quantum treatment can also be applied to the study of the photodissociation of an arbitrary diatomic molecule in ^4He_N.

Comparing the catalytic activity of the water gas shift reaction on Cu(321) and Cu(111) surfaces: step sites do not always enhance the overall reactivity

H. Prats, P. Gamallo, F. Illas, R. Sayós.

J. Cat., 342 (2016) 75.



A Density Functional Theory based first-principles kinetic Monte Carlo (kMC) study of the water gas shift reaction on the stepped Cu(321) surface is presented. We use the recently developed graph-theoretical kMC approach coupled with cluster expansion Hamiltonians to model the coverage-dependent energy barriers for the different surface processes, including adsorption/desorption, diffusion and other elementary chemical reactions, totalling 36 elementary steps, which allow two possible competitive mechanisms: surface redox and associative COOH. All results are compared to a previous kMC study on Cu(111). Both mechanisms are observed for Cu(321) surface with different extension, whereas the associative COOH one was the dominant for Cu(111). The present study shows that, in spite of encompassing lower activation energy barriers, stepped surfaces do not necessarily have an overall larger catalytic activity. Coverage effects and the significant contribution of some of the reverse processes are behind this behaviour.

III.2 PUBLICATION LIST

PUBLISHED ARTICLES

1. *Functionalized surfaces with tailored wettability determine influenza A infectivity.*
I. Mannelli, R. Reigada, I. Suárez, D. Janner, A. Carrilero, P. Mazumder, F. Sagués, V. Pruneri, M. Lakadamyali.
ACS Appl. Mater. Interfaces *8* (2016) 15058.

2. *Highly versatile polyelectrolyte complexes for improving the enzyme replacement therapy of lysosomal storage disorders.*
M. I. Giannotti, I. Abasolo, M. Oliva, F. Andrade, N. Garcia-Aranda, M. Melgarejo, D. Pulido, J. L. Corchero, Y. Fernandez, A. Villaverde, M. Royo, M. F. Garcia-Parajo, F. Sanz, S. Schwartz.
ACS Appl. Mater. Interfaces *8* (2016) 25741.

3. *The interplay between homogeneous and heterogeneous phases of PdAu catalysts for the oxidation of alcohols.*
J. Jover, M. García-Ratés, N. López.
ACS Catal. *6* (2016) 4135.

4. *A β-mannannase with a lysozyme fold and a novel molecular catalytic mechanism.*
Y. Jin, M. Petricevic, A. John, L. Raich, H. Jenkins, L. Portela De Souza, F. Cuskin, H. J. Gilbert, C. Rovira, E. D. Goddard-Borger, S. J. Williams, G. J. Davies.
ACS Cent. Sci. *2* (2016) 896.

5. *Sequential electron transport and vibrational excitations in an organic molecule coupled to few-layer graphene electrodes.*
E. Burzuri, J. O. Island, R. Diaz-Torres, A. Fursina, A. Gonzalez-Campo, O. Roubeau, S. J. Teat, N. Aliaga-Alcalde, E. Ruiz, H. S. J. van der Zant.
ACS Nano *6* (2016) 2521.

6. *Tuning crystal ordering, electronic structure, and morphology in organic semiconductors: tetrathiafulvalenes as a model case.*
R. Pfattner, S. T. Bromley, C. Rovira, M. Mas-Torrent.
Adv. Funct. Mat. *26* (2016) 2256.

7. *Force-induced reversal of ß-eliminations: stressed disulfide bonds in alkaline solution.*
P. Dopieralski, J. Ribas-Ariño, P. Anjukandi, M. Krupicka, D. Marx.
Angew. Chem. Int. Ed. *55* (2016) 1304.

8. *High efficiency of Pt^{2+} - CeO_2 novel thin film catalyst as anode for proton exchange membrane fuel cells.*
R. Fiala, A. Figueroba, A. Bruix, M. Vaclavu, A. Rednyk, I. Khalakhan, M. Vorokhta, J. Lavkova, F. Illas, V. Potin, I. Matolinova, K. M. Neyman, V. Matolín.
Appl. Catal. B – Environ. *197* (2016) 262.

9. *Surface composition of magnetron sputtered Pt-Co thin film catalyst for proton exchange membrane fuel cells.*
M. Vorokhta, I. Khalakhan, M. Václavu, G. Kovács, S. M. Kozlov, P. Kúš, T. Skála, N. Tsud, J. Lavková, V. Potin, I. Matolínová, K. M. Neyman, V. Matolín.
Appl. Surf. Sci. *365* (2016) 245.

10. *Dust formation in the oxygen-rich AGB star IK Tauri.*
D. Gobrecht, I. Cherchneff, A. Sarangi, J. M. C. Plane, S. T. Bromley.
Astronomy & Astrophysics *585* (2016) A6.

11. *The reaction mechanism of retaining glycosyltransferases.*
A. Ardèvol, J. Iglesias-Fernández, V. Rojas-Cervellera, C. Rovira.
Biochem. Soc. Transac. *44* (2016) 51.

12. *First-principles study of structural, elastic and electronic properties of alpha-, beta- and gamma-graphyne.*
A. Ruiz-Puigdollers, G. Alonso, P. Gamallo.
Carbon *96* (2016) 879.

13. *Role of structural symmetry breaking in the structurally induced robust superlubricity of graphene and h-BN homo- and heterojunctions.*
N. Ansari, F. Nazari, F. Illas.
Carbon *96* (2016) 911.

14. *Modeling ceria-based nanomaterials for catalysis and related applications.*
A. Bruix, K. M. Neyman.
Catal. Lett. *146* (2016) 2053.

15. *Towards stable single-atom catalysts: strong binding of atomically dispersed transition metals on the surface of nanostructured ceria.*
A. Figueroba, G. Kovács, A. Bruix, K. M. Neyman.
Catal. Sci. Technol. *6* (2016) 6806.

16. *Reaction mechanism and regioselectivity of the Bingel-Hirsch addition of dimethyl bromomalonate to La@C_{2v}-C_{82}.*
J. P. Martínez, M. Garcia-Borràs, S. Osuna, J. Poater, F. M. Bickelhaupt, M. Solà.
Chem. Eur. J. *22* (2016) 5953.

17. *Hückel's rule of aromaticity categorizes aromatic closo boron hydride clusters.*
J. Poater, M. Solà, C. Viñas, F. Teixidor.
Chem. Eur. J. *22* (2016) 7437.

18. *The tetracyanopyridinide dimer dianion, σ-$[TCNPy]_2^{2-}$.*
J. Hao, A. L. Rheingold, M. Kavand, K. J. van Schooten, C. Boehme, M. Capdevila-Cortada, J. J. Novoa, E. Woss, G. Knor, J. S. Miller.
Chem. Eur. J. *22* (2016) 12312.

19. *Electronic structure modulation in an exceptionally stable non-heme nitrosyl iron(II) spin-crossover complex.*
L. Piñeiro-López, N. Ortega-Villar, M. C. Muñoz, G. Molnár, J. Cirera, R. Moreno-Esparza, V. M. Ugalde-Saldívar, A. Bousseksou, E. Ruiz, J. A. Real.
Chem. Eur. J. *22* (2016) 12741.

20. *Rational design of lanthanoid single-ion magnets: predictive power of the theoretical Models.*
J. J. Baldovi, Y. Duan, R. Morales, A. Gaita-Ariño, E. Ruiz, E. Coronado.
Chem. Eur. J. *22* (2016) 13532.

21. *Lanthanide tetrazolate complexes combining single-molecule magnet and luminescence properties: the effect of the replacement of tetrazolate N3 by β-diketonate ligands on the anisotropy energy barrier.*
J.-R. Jimenez, I. F. Diaz-Ortega, E. Ruiz, D. Aravena, S. J. A. Pope, E. Colacio, J. M. Herrera.
Chem. Eur. J. *22* (2016) 14548.

22. *Redox-assisted self-assembly of a water-soluble cyanido-bridged mixed valence $\{Co^{III}/Fe^{II}\}_2$ square.*
L. Alcázar, G. Aullón, M. Ferrer, M. Martínez.
Chem. Eur. J. *22* (2016) 15227.

23. *Formation of long, multicenter π-$[TCNE]_2^{2-}$ dimers in solution: solvation and stability assessed through molecular dynamics simulations.*
M. Capdevila-Cortada, J. Ribas-Ariño, A. Chaumont, G. Wipff, J.J. Novoa.
Chem. Eur. J. *22* (2016) 17037.

24. *Formation of a trifluorophosphane platinum(II) complex by P-F bond activation and phosphorus pentafluoride with a Pt^0 complex.*
N. Arnold, R. Bertermann, F. M. Bickelhaupt, H. Braunschweig, M. Drisch, M. Finze, F. Hupp, J. Poater, J. A. P. Sprenger.
Chem. Eur. J. *accepted* doi: 10.1002/chem.201604997

25. *A push-pull organic dye with a quinoidal thiophene linker: photophysical properties and solvent effects.*
C. Climent, A. Carreras, P. Alemany, D. Casanova.
Chem. Phys. Lett. *663* (2016) 45.

26. *From widely accepted concepts in coordination chemistry to inverted ligand fields.*
R. Hoffmann, S. Alvarez, C. Mealli, A. Falceto, T. J. Cahill, T. Zeng, G. Manca.
Chem. Rev. *116* (2016) 8173.

27. *Multiscale study of mononuclear Co-II SMMs based on curcuminoid ligands.*
R. Diaz-Torres, M. Menelaou, O. Roubeau, A. Sorrenti, G. Brandariz-de-Pedro, E. C. Sanudo, S. J. Teat, J. Fraxedas, E. Ruiz, N. Aliaga-Alcalde.
Chem. Sci. *7* (2016) 2793.

28. *Violation of DNA neighbor exclusion principle in RNA recognition.*
M. Yousuf, I. S. Youn, J. Yun, L. Rasheed, R. Valero, G. Shi, K. S. Kim.
Chem. Sci. *7* (2016) 3581.

29. *A low spin manganese(IV) nitride single molecule magnet.*
M. Ding, G. E. Cutsail Iii, D. Aravena, M. Amoza, M. Rouzieres, P. Dechambenoit, Y. Losovyj, M. Pink, E. Ruiz, R. Clérac, J. M. Smith.
Chem. Sci. *7* (2016) 6132.

30. *Design of multi-functional 2D open-shell organic networks with mechanically controllable properties.*
I. Alcón, D. Reta, I. de P. R. Moreira, S. T. Bromley.
Chem. Sci. *accepted* doi: 10.1039/C6SC01412G

31. *Exploring the origin of 'aggregation induced emission' activity and 'crystallization induced emission' in organometallic iridium(III) cationic complexes: influence of counterions.*
P. Alam, C. Climent, G. Kaur, D. Casanova, A.R. Choudhury, A. Gupta, P. Alemany, I. R. Laskar.
Cryst. Growth Des. *16* (2016) 5738.

32. *Structural and electronic characterisation of pi-extended tetrathiafulvalene derivatives as active components in field-effect transistors.*
A. Campos, N. Oxtoby, S. Galindo, R. Pfattner, J. Veciana, S. T. Bromley, C. Rovira, M. Mas-Torrent.
CrystEngComm *18* (2016) 6149.

33. *Redox flexibility of iron complexes supported by sulfur-based tris(o-methylenethiophenolato)amine relative to its tripodal oxygen-based congener.*
A. Mondragón, P. R. Martínez-Alanis, G. Aullón, S. Hernández-Ortega, E. Robles-Marín, M. Flores-Alamo, V. M. Ugalde-Saldívar, I. Castillo.
Dalton Trans. *45* (2016) 9996.

34. *Magnetic and transport properties of Fe_4 single-molecule magnets: a theoretical insight.*
N. Gallego-Planas, A. Martin-Rodriguez, E. Ruiz.
Dalton Trans. *45* (2016) 18867.

35. *Transition metal carbides as novel materials for CO_2 capture, storage, and activation.*
C. Kunkel, F. Viñes, F. Illas.
Energy Environ. Sci. *9* (2016) 141.

36. *Synthesis and hydrolysis of alkoxy(aminoalkyl)diorganylsilanes of the formula type $R_2(RO)Si(CH_2)_nNH_2$ (R = Alyl, n = 1-3): a systematic experimental and computational study.*
J. Ehbets, S. Lorenzen, C. Mahler, R. Bertermann, A. Berkefeld, J. Poater, E. Fritz-Langhals, R. Weidner, F. M. Bickelhaupt, R. Tacke.
Eur. J. Inorg. Chem. (2016) 1641.

37. *First-principles analysis of the charge transfer in the NMP-TCNQ molecular metal and $(NMP)_x(Phen)_{1-x}TCNQ$ solid solutions.*
P. Alemany, E. Canadell, J.-P. Pouget.
Europhys. Lett. *113* (2016) 27006.

38. *Sequential measurement of displacement and conduction currents in electronic devices.*
G. Albareda, F. L. Traversa, A. Benali.
Fluct. Noise Lett. *15* (2016) 1640004.

39. *Theoretical modeling of the ligand-tuning effect over the transition temperature in four-coordinated Fe(II) molecules.*
J. Cirera, E. Ruiz.
Inorg. Chem. *55* (2016) 1657.

40. *Non-switching 1,2-dithienylethene-based diplatinum(II) complex showing high cytotoxicity.*
A. Presa, L. Barrios, J. Cirera, L. Korrodi-Gregório, R. Pérez-Tomás, S. J. Teat, P. Gamez.
Inorg. Chem. *55* (2016) 5356.

41. *Single-molecule magnet properties of transition-metal ions encapsulated in lacunary polyoxometalates: a theoretical study.*
D. Aravena, D. Venegas-Yazigi, E. Ruiz.
Inorg. Chem. *55* (2016) 6405.

42. *Predetermined ferromagnetic coupling via strict control of M-O-M angles.*
M. Fondo, J. Doejo, A. M. Garcia-Deibe, J. Sanmartin-Matalobos, R. Vicente, M. S. El-Fallah, M. Amoza, E. Ruiz.
Inorg. Chem. *55* (2016) 11707.

43. *Ferromagnetism in polynuclear systems based on non-linear $[Mn^{II}_2Mn^{III}]$ building blocks.*
J. Cirera, Y. Jiang, L. Qin, Y.-Z. Zheng, G. Li, G. Wu, E. Ruiz.
Inorg. Chem. Front. *3* (2016) 1272.

44. *A trapped covalent intermediate of a glycoside hydrolase on the pathway to transglycosylation. Insights from experiments and quantum mechanics/molecular mechanics simulations.*
L. Raich, V. Borodkin, W. Fang, J. Castro-López, D. van Aalten, R. Hurtado-Guerrero, C. Rovira.
J. Am. Chem. Soc. *138* (2016) 3325.

45. *Helical folding-induced stabilization of ferromagnetic polyradicals based on triarylmethyl radical derivatives.*
D. Reta, I. de P. R. Moreira, F. Illas.
J. Am. Chem Soc. *138* (2016) 5271.

46. *Molecular mechanisms of spin crossover in the $\{Fe(pz)[Pt(CN)_4]\}$ metal-organic framework upon water adsorption.*
C. H. Pham, J. Cirera, F. Paesani.
J. Am. Chem. Soc. *138* (2016) 6123.

47. *Localization versus delocalization in chiral single component conductors of gold bis(dithiolene) complexes.*
D.G. Branzea, F. Pop, P. Auban-Senzier, R. Clérac, P. Alemany, E. Canadell, N. Avarvari.
J. Am. Chem. Soc. *138* (2016) 6838.

48. *Highly active Au/delta-MoC and Cu/delta-MoC catalysts for the conversion of CO_2: the metal/C ratio as a key factor defining activity, selectivity, and stability.*
S. Posada-Pérez, P. J. Ramírez, J. Evans, F. Viñes, P. Liu, F. Illas, J. A. Rodriguez.
J. Am. Chem. Soc. *138* (2016) 8269.

49. *Structure of the reduced copper active site in pre-processed galactose oxidase: ligand tuning for one-electron O_2 activation in cofactor biogenesis.*
R. E. Cowley, J. Cirera, M. F. Qayyum, D. Rokhsana, B. Hedman, K. O. Hodgson, D. M. Dooley, E. I. Solomon.
J. Am. Chem. Soc. *138* (2016) 13219.

50. *Relaxation dynamics of identical trigonal bipyramidal cobalt molecules with different local symmetries and packing arrangements: magnetostructural correlations and ab initio calculations.*
T. J. Woods, M. F. Ballesteros-Rivas, S. Gomez-Coca, E. Ruiz, K. R. Dunbar.
J. Am. Chem. Soc. *138* (2016) 16407.

51. *Kinetic Monte Carlo simulations of the water gas shift reaction on Cu(111) from density functional theory based calculations.*
H. Prats, L. Álvarez, F. Illas, R. Sayós.
J. Catal. *333* (2016) 217.

52. *Insights from methane decomposition on nanostructured palladium.*
S. M. Kozlov, K. M. Neyman.
J. Catal. *337* (2016) 111.

53. *Comparing the catalytic activity of the water gas shift reaction on Cu(321) and Cu(111) surfaces: step sites do not always enhance the overall reactivity.*
H. Prats, P. Gamallo, F. Illas, R. Sayós.
J. Catal. *342* (2016) 75.

54. *Effects of electron transfer in model catalysts composed of Pt nanoparticles on CeO_2(111) surface.*
S. M. Kozlov, K. M. Neyman.
J. Catal. *344* (2016) 507.

55. *Assessment of the sampling performance of multiple-copy dynamics versus a unique trajectory.*
J. J. Pérez, M. S. Tomas, J. Rubio-Martinez.
J. Chem. Inf. Model. *56* (2016) 1950.

56. *Consequences of electron correlation for XPS binding energies: Representative case for C(1s) and O(1s) XPS of CO.*
P. S. Bagus, C. Sousa, F. Illas.
J. Chem. Phys. *145* (2016) 144303.

57. *Performance of the TPSS functional on predicting core level binding energies of main group elements containing molecules: a good choice for molecules adsorbed on metal surfaces.*
N. Pueyo-Bellafont, F. Viñes, F. Illas.
J. Chem. Theo. Comput. *12* (2016) 324.

58. *Effect of the exchange-correlation potential on the transferability of Brønsted-Evans-Polanyi relationships in heterogeneous catalysis.*
J. L. C. Fajín, F. Viñes, M. N. D. S. Cordero, F. Illas, J. R. B. Gomes.
J. Chem. Theo. Comput. *12* (2016) 2121.

59. *Magnetic coupling constants in three electrons three centers problems from effective hamiltonian theory and validation of broken symmetry-based approaches.*
D. Reta, I. de P. R. Moreira, F. Illas.
J. Chem. Theo. Comput. *12* (2016) 3228.

60. *Effect of size and structure on the ground-state and excited-state electronic structure of TiO_2 nanoparticles.*
D. Cho, K. C. Ko, O. Lamiel-Garcia, S. T. Bromley, J. Y. Lee, F. Illas.
J. Chem. Theo. Comput. *12* (2016) 3751.

61. *On the zeroth-order hamiltonian for CASPT2 calculations of spin crossover compounds.*
S. Vela, M. Fumanal, J. Ribas-Ariño, V. Robert.
J. Comput. Chem. *37* (2016) 947.

62. *Complexes of adamantane-based groups 13 Lewis acids and superacids: bonding analysis and thermodynamics of hydrogen splitting.*
M. El-Hamdi, M. Solà, J. Poater, A. T. Timoshkin.
J. Comput. Chem. *37* (2016) 1355.

63. *Reaction rates in a theory of mechanochemical pathways.*
W. Quapp, J. M. Bofill.
J. Comput. Chem. *37* (2016) 2467.

64. *Analyzing slowly exchanging protein conformations by ion mobility mass spectrometry: study of the dynamic equilibrium of prolyl oligopeptidase.*
A. López, M. Vilaseca, S. Madurga, M. Varese, T. Tarragó, E. Giralt.
J. Mass Spectrom. *5* (2016) 504-511.

65. *Boron oxide glasses and nanocomposites: synthetic, structural and statistical approach.*
H. Hristov, M. Nedyalkova, S. Madurga, V. Simeonov.
J. Mater. Sci. Technol. *accepted* doi: 10.1016/j.jmst.2016.07.016

66. *From the LiI-$(CH_3CN)_{1-10}$ small clusters to the solvation process in acetonitrile solutions of lithium iodide.*
M. Albertí, A. Amat, F. De Angelis, F. Pirani.
J. Mol. Liq. *218* (2016) 294.

67. *Aqueous N-methylacetamide new analytic potentials and a molecular dynamics study.*
N. Faginas-lago, A. Lombardi, M. Albertí.
J. Mol. Liq. *224* (2016) 792.

68. *Synthesis, characterization, crystal structures and computational studies on novel cyrhetrenyl hydrazones.*
J. Gómez, N. Leiva, R. Arancibia, J. Oyarzo, G. E. Buono-Core, A. H. Klahn, V. Artigas, M. Fuentealba, R. Bosque, G. Aullón, C. López, M. Font-Bardía, T. Calvet
J. Organomet. Chem. *819* (2016) 129-137.

69. *Molecular dynamics simulations of small clusters and liquid hydrogen sulfide at different thermodynamic conditions.*
M. Albertí, A. Amat, A. Aguilar; F. Pirani.
J. Phys. Chem. A *120* (2016) 4749.

70. *Dehydrohalogenation and dehydration reactions of i-C_3H_7Br and i-C_3H_7OH by sodium ions studied by guided ion beams techniques and quantum chemical methods.*
E. López, J. M. Lucas, J. de Andrés, M. Albertí, J. M. Bofill, A. Aguilar.
J. Phys. Chem. A *120* (2016) 4758.

71. *Adsorption of hydrogen molecules on carbon nanotubes using quantum chemistry and molecular dynamics.*
N. Faginas-Lago, D. Yeni, F. Huarte, Y. Wang, M. Alcamí, F. Martin.
J. Phys. Chem. A *120* (2016) 6451.

72. *Diffusion of H_2 and D_2 confined in single-walled carbon nanotubes: quantum dynamics and confinement effects.*
M. Mondelo-Martell, F. Huarte-Larrañaga.
J. Phys. Chem. A *120* (2016) 6501.

73. *Near-edge X-ray absorption fine structure investigation of the quasi-one-dimensional organic conductor $(TMTSF)_2PF_6$.*
K. Medjanik, A. Chernenkaya, X. Kozina, S. A. Nepijko, G. Öhrwall, P. Foury-Leylekian, P. Alemany, G. Schönhense, E. Canadell, J.-P. Pouget.
J. Phys. Chem. A *120* (2016) 8574.

74. *Reaction coordinates and pathways of mechanochemical transformations.*
W. Quapp, J. M. Bofill.
J. Phys. Chem. B *120* (2016) 2644.

75. *Structure and properties of zirconia nanoparticles from density functional theory calculations.*
A. Ruiz-Puigdollers, F. Illas, G. Pacchioni.
J. Phys. Chem. C *120* (2016) 4392.

76. *Atomically dispersed Pd, Ni and Pt species in ceria-based catalysts: Principal differences in stability and reactivity.*
A. Neitzel, A. Figueroba, Y. Lykhach, T. Skála, M. Vorokhta, N. Tsud, S. Mehl, K. Ševcíková, K. C. Prince, K. M. Neyman, V. Matolín, J. Libuda.
J. Phys. Chem. C *120* (2016) 9852.

77. *Effect of nanostructuring on the reactivity of zirconia: a DFT plus U study of Au atom adsorption.*
A. Ruiz-Puigdollers, F. Illas, G. Pacchionni.
J. Phys. Chem. C *120* (2016) 17604.

78. *Stabilization of small platinum nanoparticles on Pt-CeO_2 thin film electrocatalysts during methanol oxidation.*
O. Brummel, F. Waidhas, F. Faisal, R. Fiala, M. Vorokhta, I. Khalakhan, M. Dubau, A. Figueroba, G. Kovács, H. A. Aleksandrov, G. N. Vayssilov, S. M. Kozlov, K. M. Neyman, V. Matolín, J. Libuda.
J. Phys. Chem. C *120* (2016) 19723.

79. *Evidence for multi-polymorphic islands during epitaxial growth of ZnO on Ag(111).*
I. Demiroglu, S. T. Bromley.
J. Phys.: Condens. Matter *28* (2016) 224007.

80. *Local energy and power in many-particle quantum systems driven by an external electrical field.*
G. Albareda, F. L. Traversa, X. Oriols.
J. Stat. Mech. Theo. Exp. *5* (2016) 054026.

81. *Lipid vesicle interaction with hydrophobic surfaces: a coarse-grained molecular dynamics study.*
I. Mannelli, F. Sagués, V. Pruneri, R. Reigada.
Langmuir *32* (2016) 12632.

82. *Disclosing the ligand- and solvent-induced changes on the spin transition and optical properties of Fe(II)-indazolylpyridine complexes.*
S. Vela, C. Gourlaouen, M. Fumanal, J. Ribas-Ariño.
Magnetochemistry *2* (2016) 6.

83. *Enzymatic cleavage of glycosidic bonds: strategies on how to setup and control a QM/MM metadynamics simulation.*
L. Raich, A. Nin-Hill, A. Ardèvol, C. Rovira.
Methods Enzymol. *577* (2016) 159.

84. *Large conductance switching in a single-molecule device through room temperature spin-dependent transport.*
A. C. Aragones, D. Aravena, J. I. Cerda, Z. Acis-Castillo, H. Li, J. A. Real, F. Sanz, J. Hihath, E. Ruiz, I. Diez-Perez
Nano Lett. *16* (2016) 218.

85. *Exchange coupling inversion in a high-spin organic triradical molecule.*
R. Gaudenzi, E. Burzuri, D. Reta, I. de P. R. Moreira, S. T. Bromley, C. Rovira, J. Veciana, H. S. J. van der Zant.
Nano Lett. *16* (2016) 2066.

86. *Electrostatic catalysis of a Diels–Alder reaction.*
A. C. Aragonès, N. L. Haworth, N. Darwish, S. Ciampi, N. J. Bloomfield, G. G. Wallace, I. Diez-Perez, M. L. Coote.
Nature *531* (2016) 88.

87. *Unexpected mechanochemical complexity in the mechanistic scenarios of disulfide bond reduction in alkaline solution.*
P. Dopieralski, J. Ribas-Ariño, P. Anjukandi, M. Krupicka, D. Marx.
Nature Chem. (2016) doi: 10.1038/nchem.2632

88. *Counting electrons on supported nanoparticles.*
Y. Lykhach, S. M. Kozlov, T. Skála, A. Tovt, V. Stetsovych, N. Tsud, F. Dvorák, V. Johánek, A. Neitzel, J. Myslivecek, S. Fabris, V. Matolín, K. M. Neyman, J. Libuda.
Nature Mater. *15* (2016) 284.

89. *Simultaneous and coordinated rotational switching of all molecular rotors in a network.*
Y. Zhang, H. Kersell, R. Stefak, J. Echeverría, V. Iancu, U. G. E. Perera, Y. Li, A. Deshpande, K.–F. Braun, C. Joachim, G. Rapenne, S.–W. Hla.
Nature Nanotechnol. *11* (2016) 706.

90. *Size and shape trump charge in interactions of oxovanadates with self-assembled interraces: application of continuous shape measure analysis to the decavanadate anion.*
I. Sanchez-Lombardo, B. Baruah, S. Alvarez, K. R. Werst, N. A. Segaline, N. E. Levinger, D. C. Crans.
New J. Chem. *40* (2016) 962.

91. *Pyridinethiolate titanocene metalloligands and their self-assembly reactions to yield early-late metallamacrocycles.*
M. Ferrer, D. Gómez-Bautista, A. Gutiérrez, G. Orduna-Marco, L. A. Oro, J. J. Pérez-Torrente, O. Rossell, E. Ruiz.
Organometallics *35* (2016) 336.

92. *Mechanistic investigation of iridium-catalyzed C–H borylation of methyl benzoate: Ligand effects in regioselectivity and activity.*
J. Jover, F. Maseras.
Organometallics *35* (2016) 3221.

93. *Selective derivatization of N-terminal cysteines using cyclopentenediones.*
O. Brun, J. Agramunt, L. Raich, C. Rovira, E. Pedroso, A. Grandas.
Org. Lett. *18* (2016) 4836.

94. *FMOC-RGDS based fibrils: atomistic details of their hierarchical assembly.*
D. Zanuy, J. Poater, M. Solà, I. Hamley, C. Alemán.
Phys. Chem. Chem. Phys. *18* (2016) 1265.

95. *Quantum dynamics of the pick up process of atoms by superfluid helium nanodroplets: the Ne + $(^4He)_{1000}$ system.*
A. Vilà, M. González, R. Mayol.
Phys. Chem. Chem. Phys. *18* (2016) 2016.

96. *Relaxation dynamics of helium nanodroplets after photodissociation of a dopant homonuclear diatomic molecule. The case of $Cl_2@(^4He)_N$.*
A. Vilà, M. González, R. Mayol.
Phys. Chem. Chem. Phys. *18* (2016) 2409.

97. *Unexpectedly large impact of van der Waals interactions on the description of heterogeneously catalyzed reactions: the water gas shift reaction on Cu(321) as a case example.*
H. Prats, P. Gamallo, R. Sayós, F. Illas.
Phys. Chem. Chem. Phys. *18* (2016) 2792.

98. *Paramagnetic spherical nanoparticles by the self-assembly of persistent trityl radicals.*
I. Marin-Montesinos, J. C. Paniagua, A. Peman, M. Vilaseca, F. Luis, S. Van Doorslaer, M. Pons.
Phys. Chem. Chem. Phys. *18* (2016) 3151.

99. *Reactivity of atomically dispersed Pt^{2+} species towards H_2: Model Pt-CeO_2 fuel cell catalysts.*
Y. Lykhach, A. Figueroba, M. F. Camellone, A. Neitzel, T. Skála, F. R. Negreiros, M. Vorokhta, N. Tsud, K. C. Prince, S. Fabris, K. M. Neyman, V. Matolín, J. Libuda.
Phys. Chem. Chem. Phys. *18* (2016) 7672.

100. *Octahedral aromaticity in $^{2S+1}A_{1g}$ X_6^q clusters (X = Li-C and Be-Si, S = 0-3, and q = -2 to +4).*
O. El-Bakouri, M. Duran, J. Poater, F. Feixas, M. Solà.
Phys. Chem. Chem. Phys. *18* (2016) 11700.

101. *Performance of a modified hybrid functional in the simultaneous description of stoichiometric and reduced TiO_2 polymorphs.*
K. C. Ko, O. Lamiel-Garcia, J. Y. Lee, F. Illas.
Phys. Chem. Chem. Phys. *18* (2016) 12357.

102. *Impact of the water dimer on the atmospheric reactivity of carbonyl oxides.*
J. M. Anglada, A. Solé.
Phys. Chem. Chem. Phys. *18* (2016) 17698.

103. *The quest for rationalizing the magnetism in purely organic semiquinone-bridged bisdithiazolyl molecular magnets.*
M. Fumanal, M. Deumal.
Phys. Chem. Chem. Phys. *18* (2016) 20738.

104. *Planar vs. three-dimensional X_6^{2-}, $X_2Y_4^{2-}$, and $X_3Y_3^{2-}$ (X, Y = B, Al, Ba) metal clusters: an analysis of their relative energies through the turn-upside-down approach.*
O. El-Bakouri, M. Solà, J. Poater.
Phys. Chem. Chem. Phys. *18* (2016) 21102.

105. *Can the state of platinum species be unambiguously determined by the stretching frequency of adsorbed CO probe molecule?*
H. A. Aleksandrov, K. M. Neyman, K. I. Hadjiivanov, G. N. Vayssilov.
Phys. Chem. Chem. Phys. *18* (2016) 22108.

106. *Single oxygen vacancies of $(TiO_2)_{35}$ as a prototype reduced nanoparticle: implication for photocatalytic activity.*
S. Kim, K. C. Ko, J. Y. Lee, F. Illas.
Phys. Chem. Chem. Phys. *18* (2016) 23755.

107. *Under what conditions does $(SiO)_N$ nucleation occur? A bottom-up kinetic modelling evaluation.*
S. T. Bromley, J. C. Gómez Martín, J. M. C. Plane.
Phys. Chem. Chem. Phys. *18* (2016) 26913.

108. *Mass effects in the photodissociation of homonuclear diatomic molecules in helium nanodroplets: inelastic collision and viscous flow energy exchange regimes.*
A. Vilà, M. González.
Phys. Chem. Chem. Phys. *18* (2016) 27630.

109. *Reaction dynamics inside superfluid helium nanodroplets: the formation of the Ne_2 molecule from Ne + Ne@(^{4}He)$_N$.*
A. Vilà, M. González.
Phys. Chem. Chem. Phys. *18* (2016) 31869.

110. *The reaction mechanism of polyalcohol dehydration in hot pressurized water.*
S. Ruiz-Barragan, J. Ribas-Ariño, M. Shiga.
Phys. Chem. Chem. Phys. *18* (2016) 32438.

111. *Universal steps in quantum dynamics with time-dependent potential-energy surfaces: beyond the born-oppenheimer picture.*
G. Albareda, A. Abedi, I. Tavernelli, A. Rubio.
Phys. Rev. A *94* (2016) 062511.

112. *Equilibrium microphase separation in the two-leaflet model of lipid membranes.*
R. Reigada, A. S. Mikhailov.
Phys. Rev. E *93* (2016) 010401(R).

113. *Atomic and molecular collisional data for spacecraft re-entry plasmas.*
R. Celiberto, I. Armenise, M. Cacciatore, M. Capitelli, F. Esposito, P. Gamallo, R. K. Janev, A. Laganà, V. Laporta, A. Laricchiuta, A. Lombardi, M. Rutigliano, R. Sayós, J. Tennyson, J. M. Wadehra.
Plasma Sources Sci. Technol. *25* (2016) 033004.

114. *Antiferro- to ferromagnetic crossover in diphenoxido bridged $Ni^{II}_2Mn^{II}$ complexes derived from N_2O_2 donor Schiff base ligands.*
P. Seth, A. Figuerola, J. Jover, E. Ruiz, A. Ghosh.
Polyhedron *117* (2016) 59.

115. *Self-assembly of discrete metallocycles versus coordination polymers based on Cu(I) and Ag(I) ions and flexible ligands: structural diversification and luminescent properties.*
J. Vallejos, I. Brito, A. Cárdenas, M. Bolte, S, Conejeros, P. Alemany, J. Llanos.
Polymers *8* (2016) 46.

116. *Steering the formation of supported Pt-Sn nanoalloys by reactive metal-oxide interaction.*
A. Neitzel, G. Kovács, Y. Lykhach, N. Tsud, S. M. Kozlov, T. Skála, M. Vorokhta, V. Matolín, K. M. Neyman, J. Libuda.
RSC Adv. *6* (2016) 85688.

117. *Fractal dimension of the trajectory of a single particle diffusing in crowded media.*
L. Pitulice, D. Craciun, E. Vilaseca, S. Madurga, I. Pastor, F. Mas, A. Isvoran.
Romanian Journal of Physics *61* (2016) 1276-1286.

118. *Exchange interactions on the highest-spin reported molecule: the mixed-valence Fe_{42} complex.*
D. Aravena, D. Venegas-Yazigi, E. Ruiz
Sci. Rep. *6* (2016) 23847.

119. *Alteration of interleaflet coupling due to compounds displaying rapid translocation in lipid membranes.*
R. Reigada.
Sci. Rep. *6* (2016) 32934.

120. *Tuning the electrical conductance of metalloporphyrin supramolecular wires.*
M. Noori, A. C. Aragonès, G. Di Palma, N. Darwish, S. W. D. Bailey, Q. Al-Galiby, I. Grace, D. B. Amabilino, A. González-Campo, I. Díez-Pérez, C. J. Lambert.
Sci. Rep. *6* (2016) 37352.

121. *How carbo-benzenes fit molecules in their inner core as do biologic ion carriers.*
F. Turias, J. Poater, R. Chauvin, A. Poater.
Struct. Chem. *27* (2016) 249.

122. *On the hydrogen adsorption and dissociation on Cu surfaces and nanorows.*
L. Álvarez-Falcón, F. Viñes, A. Notario-Estevez, F. Illas.
Surf. Sci. *646* (2016) 221.

123. *DFT approaches to transport calculations in magnetic single-molecule devices.*
A. Martín-Rodríguez, D. Aravena, E. Ruiz.
Theor. Chem. Acc. *135* (2016) 1.

124. *The variational nature of the gentlest ascent dynamics and the relation of a variational minimum of a curve and the minimum energy path.*
J. M. Bofill, W. Quapp.
Theor. Chem. Acc. *134* (2016) 11.

125. *Performance of Minnesota functionals on predicting core-level binding energies of molecules containing main-group elements.*
N. Pueyo-Bellafont, G. Alvarez-Saiz, F. Viñes, F. Illas.
Theor. Chem. Acc. *135* (2016) 35.

126. *A contribution to a theory of mechanochemical pathways by means of Newton trajectories.*
W. Quapp, J. M. Bofill.
Theor. Chem. Acc. *135* (2016) 113.

127. *A force field for acetone: the transition from small clusters to liquid phase investigated by molecular dynamics simulations.*
N. Faginas-Lago, M. Albertí, A. Lombardi.
Theor. Chem. Acc. *135* (2016) 161.

128. *The contact of graphene with Ni(111) surface: description by modern dispersive forces approaches.*
H. Muñoz-Galán, F. Viñes, J. Gebhardt, A. Görling, F. Illas.
Theor. Chem. Acc. *135* (2016) 165.

129. *Exploring the validity of the Glidewell-Lloyd extension of Clar's pi-sextet rule: assessment from polycyclic aromatic hydrocarbons.*
O. El-Bakouri, J. Poater, F. Feixas, M. Solà.
Theor. Chem. Acc. *135* (2016) 205.

BOOK CHAPTERS AND PROCEEDINGS

1. *QM/MM calculations on selectivity in homogeneous catalysis*
   J. Jover, F. Maseras.
   Structure and Bonding *167* (2016) 59

2. *Comparison of the Cr-Cr quadruple and quintuple bonding mechanisms*
   A. Falceto, S. Alvarez.
   Structure and Bonding *170* (2016) 249

3. *Modeling Magnetic Properties with Density Functional Theory-Based Methods*
   J. Cirera, E. Ruiz.
   Molecular Magnetic Materials edited by B. Sieklucka and D. Pinkowicz (2016), 417, Wiley-VCH.

4. *Ab Initio Wavefunction Approaches to Spin States*
   C. Sousa, C. de Graaf.
   Spin States in Biochemistry and Inorganic Chemistry. Influence on Structure and Reactivity (2016) Wiley**.**

5. *An Application of the Maximum Principle in Chemistry: A Method to Locate Transition States*
   J. M. Bofill, W. Quapp.
   Theoretical & Quantum Chemistry at the Dawn's End of 21st Century edited by R. Carbó-Dorca and T. Chakraborty (2016) Taylor & Francis Group, London.

6. *Electron Devices Simulation with Bohmian Trajectories*
   G. Albareda, D. Marian, A. Benali, A. Alarcón, S. Moises, X. Oriols.
   Simulation of Transport in Nanodevices edited by F. Triozon and P. Dollfus (2016) ISTE Ltd., Wiley & Sons Inc.

7. *Rules of aromaticity*
   F. Feixas, E. Matito, J. Poater, M. Solà.
   Challenges and advances in computational chemistry and physics edited by R. Chauvin, C. Lepetit, B. Silvi and E. Alikhani (2016) Springer.

8. *QM/MM simulations of Au nanoclusters and glutathione ligands in water solvent*
   V. Rojas-Cervellera, C. Rovira, J. Akola.
   Proceedings of the 16th International Conference on Computational and Mathematical Methods in Science and Engineering, CMMSE (2016).

9. *Unraveling enzymatic mechanisms by means of computational tools: biotechnological implications in the study of glycosidases*
   L. Raich, C. Rovira.
   Revista de la Societat Catalana de Química *15* (2016) 9.

10. *Modeling reactivity in metalloproteins: hydrogen peroxide decomposition by heme enzymes*
M. Alfonso-Prieto, C. Rovira.
Simulating Enzyme Reactivity, *15* (2016) 453 Royal Society of Chemistry, Cambridge.

11. *Acetone clusters Molecular Dynamics using a semiempirical intermolecular potential*
N. Faginas-Lago, M. Albertí, A. Lombardi.
Lecture Notes in Comput. Sci. *9786* (2016) 129.

III.3 OTHER ACTIVITIES

DOCTORALS THESES 2016

1. *Estudio teórico de enlaces no clásicos.*
   Andrés Falceto Palacín
   Supervisor/s: S. Alvarez.
   Molecular Inorganic Chemistry PhD programme.
   Faculty of Chemistry, University of Barcelona.
   December 2016.

2. *Computational Study of the Mechanisms that Stabilize Organic Molecule-Based Magnets.*
   Maria Pilar Lafuente Hernández
   Supervisor/s: M. Deumal, J. J. Novoa.
   Theoretical and Computational Chemistry PhD programme.
   Faculty of Chemistry, University of Barcelona.
   December 2016.

3. *Understanding and predicting magnetic coupling in complex systems: from inorganic complexes to organic polyradicals.*
   Daniel Reta Mañeru
   Supervisor/s: I. de P. R. Moreira, F. Illas.
   Theoretical and Computational Chemistry PhD programme.
   Faculty of Chemistry, University of Barcelona.
   January 2016.

MASTERS THESES 2016

1. *Catalytic reaction of β-galactocerebrosidase investigated by QM/MM ab initio metadynamics*
   Alba Nin Hill
   Supervisor/s: C. Rovira.
   European Master in Theoretical Chemistry and Computational Modelling.
   Faculty of Chemistry, University of Barcelona.
   July 2016.

2. *Single-molecule electronic transport through transition metal complexes.*
   Alejandro Martín Rodríguez
   Supervisor/s: E. Ruiz.
   European Master in Theoretical Chemistry and Computational Modelling.
   Faculty of Chemistry, University of Barcelona.
   July 2016.

3. *Toward a drug design that selective activate the pro-apoptotic bax protein using multiple representative structures.*
Anna Cebrián Prats
Supervisor/s: J. Rubio.
European Master in Theoretical Chemistry and Computational Modelling.
Faculty of Chemistry, University of Barcelona.
July 2016.

4. *Estudi del rendiment i aplicabilitat del Force Field FFSiOH per a clústers de silica amb diferents graus d'hidroxilació.*
Antoni Macià Escatllar
Supervisor/s: S. Bromley.
European Master in Theoretical Chemistry and Computational Modelling.
Faculty of Chemistry, University of Barcelona.
July 2016.

5. *Study of the spin interactions and magnetism in $Cu(hfac)_2L^R$ (L^R=butil-pirazolyl nitronyl nitroxide) "breathing crystal".*
Cristina Roncero Barrero
Supervisor/s: M. Deumal.
Master in Atomistic and Multiscale Computational Modelling in Physics, Chemistry and Biochemistry.
Faculty of Chemistry, University of Barcelona.
July 2016.

6. *Conditional Wave Function approach to ab-initio molecular and electron dynamics.*
Efrem Bernuz Fitó
Supervisor/s: G. Albareda, J. M. Bofill.
European Master in Theoretical Chemistry and Computational Modelling.
Faculty of Chemistry, University of Barcelona.
July 2016.

7. *Estudio computacional del efecto del disolvente en la transición de espín de los sistemas $[Fe(E\text{-}dpsp)_2](BF_4)_2$·acetona y $[Fe(E\text{-}dpsp)_2](BF_4)_2$·PC*
Fernando Jiménez Grávalos
Supervisor/s: J. Ribas.
European Master in Theoretical Chemistry and Computational Modelling.
Faculty of Chemistry, University of Barcelona.
July 2016.

8. *Modelització de l'intermedi de reacció en quitinases.*
Joan Coines López-Nieto
Supervisor/s: C. Rovira, X. Biarnés.
Master in Bioengineering.
Institut Químic de Sarrià, Ramon Llull University.
July 2016.

9. *Development of a Brownian Dynamics simulation code for enzymatic reaction-diffusion processes in cowded intracellular environments.*
Mireia Via Nadal
Supervisor/s: S. Madurga, F. Mas.
European Master in Theoretical Chemistry and Computational Modelling.
Faculty of Chemistry, University of Barcelona.
July 2016.

10. *The effect of macromolecular crowding on oligomeric enzyme kinetics: Negative cooperativity on GDH.*
Núria Vilaplana Lopera
Supervisor/s: F. Mas, C. Balcells.
Master in Molecular Biotechnology.
Faculty of Pharmacy, University of Barcelona.
July 2016.

11. *Brownian Dynamics simulation of macromolecule diffusion in intracellular media.*
Pablo M. Blanco Andrés
Supervisor/s: S. Madurga.
Master in Atomistic and Multiscale Computational Modelling in Physics, Chemistry and Biochemistry.
Faculty of Chemistry, University of Barcelona.
July 2016.

SCIENTIFIC CONFERENCES AND MEETINGS 2016

251st ACS National Meeting & Exposition - Computers in Chemistry
San Diego (USA), 13 – 17 march 2016

Aromaticity criteria based on electron delocalization measures (oral communication)
J. Poater

Role of hydrogen bonding, pi-pi stacking interactions, twist angle, and solvation on B-DNA (oral communication)
J. Poater

Close connection between pi aromaticity of hydrocarbons and three-dimensional aromaticity of closo boron hydrides (oral communication)
J. Poater

252nd ACS National Meeting & Exposition – Chemistry of the people, by the people, for the people
Philadelphia (USA), 21 – 25 august 2016

How carbohydrate active enzymes work. Insights from QM/MM simulations oral communication)
C. Rovira

2nd Advances in Crystal Engineering
Barcelona (Spain), 15 january 2016

J. J Novoa (*meeting organizer*)

1st Aerospace Thematic Workshop EUCASS - Fundamentals of Collisions of Fast Particles with Surfaces – ATW2016
Aussois (France), 11 – 16 september 2016

Gas surface processes on re-entry heat shields (invited talk)
P. Gamallo

67th Annual Meeting of the International Society of Electrochemistry
The Hague (Netherlands), 21 – 26 august 2016

Studying chemical reactions at the nanoscale (oral communication)
A. C. Aragonès, N. Darwish, S. Ciampi, M. Coote, I. Díez-Pérez

Studying charge transport in Single-Protein wires (oral communication)
M. Pozuelo-Ruiz, J. M. Artés, F. Sanz, P. Gorostiza, I. Díez-Pérez

Annual User Meeting of the Spanish Supercomputing Network (Red Española de Supercomputación)
León (Spain), 20 september 2016

Computational design of advanced nanoalloy materials (invited talk)
K. M. Neyman, G. Kovács, S. M. Kozlov

CECAM Workshop: Different Routes to Quantum Molecular Dynamics
Lausanne (Switzerland), 6 – 10 june 2016

G. Albareda (*meeting organizer*)

Towards ab-initio molecular dynamics without Born-Oppenheimer potential-energy surfaces (*oral communication*)
G. Albareda, A. Abedi, I. Tavernelli, A. Rubio

CECAM Workshop: Towards a Common Format for Computational Materials Science Data
Laussane (Switzerland), 25 january – 5 february 2016

Additional properties a quantum chemist will like to find in NOMAD (oral communication)
F. Illas

CECAM Workshop: Structure prediction of nanoclusters from global optimization techniques: computational strategies and connection to experiments
Pau (France), 5 – 8 july 2016

Global optimisation of silicon oxide clusters (oral communication)
S. T. Bromley

IV Congreso Nacional de Nanotecnología 2016
Olmué (Chile), 5 – 7 september 2016

Probing new concepts in single-molecule wires: diode, electromechanics, transistor, magnetoresistance, photoswitching and chemical reactivity (oral communication)
I. Díez-Pérez

EMRS 2016 Spring Meeting
Lille (France), 2 – 6 may 2016

Design of open-shell 2D covalent materials with controllable properties (oral communication)
S. T. Bromley, I. Alcón

4th Energy Materials Workshop of the Thomas Young Centre and TOUCAN International conference Shaping Nanocatalysts
London (UK), 14 – 16 december 2016

Sophisticated computational design of bimetallic nanocrystallites (invited talk)
K. M. Neyman, G. Kovács, S. M. Kozlov

K. M. Neyman (*chairman*)

ESPA2016: 10th Congress on Electronic Structure: Principles and Applications
Castelló de la Plana (Spain), 28 june – 1 july 2016

On the mechanism of bistability in molecule-based magnets: the prototype PDTA case (poster)
T. Francese, M. Deumal, J. Ribas-Ariño, J.J. Novoa

How carbohydrate-active enzymes work (oral communication)
C. Rovira

6th EuCheMS Chemistry Congress
Sevilla (Spain), 11-15 september 2016

Selective capture and separation of industrial post-combustion gases using zeolites: a theoretical approach (poster)
H. Prats, G. Alonso, D. Bahamón, X. Giménez, R. Sayós, P. Gamallo

Effect of impurities in CO_2 capture with Mg-MOF-74 and their role in swing adsorption processes (poster)
X. Giménez, F. Keshavarz, D. Bahamón, P. Gamallo, R. Sayós

Kinetic Monte Carlo study of the water gas shift reaction on Cu (321) surface based on density functional theory data (oral keynote)
R. Sayós, H. Prats, P. Gamallo, F. Illas

Dihydrogen interactions in alkanes (oral communication)
J. Echeverría

Aromaticity: A complex concept which may be made understood to the public (oral communication)
M. Duran, S. Simon, M. Solà, J. Poater

1st European Conference of Molecular Spintronics
Bologna (Italy), 15-18 november 2016

Magnetoresistance in single-molecule devices based on magnetic mononuclear transition metal complexes (oral communication)
E. Ruiz

European Conference on Laboratory Astrophysics – Gas on the Rocks - ECLA 2016
Madrid (Spain), 21 – 25 november 2016

Silicate dust: a bottom-up computational approach (oral communication)
S. T. Bromley

21st European Conference on the Dynamics of Molecular Systems - MOLEC 2016
Toledo (Spain), 11 – 16 september 2016

Environmentally relevant ion-molecule processes: Non-adiabatic collisions in ground state N_2O and CO molecules with Na^+ and Li^+ in the 0,10-5,00 keV energy range (poster)
J. de Andrés, J. M. Lucas, M. Albertí, J. M. Bofill, A. Aguilar

Radio Frequency Ion Beams (RF-GIB) study of ion-molecule reactions having environmental, astrochemical and prebiotical relevance at the few eV energy range (poster)
J. M. Lucas, J. de Andrés, M. Albertí, J. M. Bofill, A. Aguilar

European Graphene Forum - EGF 2016
Paris (France), 1-3 june 2016

Graphynes: from competitors to graphene to atomic sieves and scatters (oral communication)
F. Viñes, M. Manadé, S. Kim, P. Gamallo, J.Y. Lee, F. Illas

Excited State Simulations: Bridging Scales workshop
Marseille (France), 7 – 10 november 2016

Computational modeling of organometallic iridium(III) triplet emitters (poster)
C. Climent, D. Casanova, P. Alemany

Fachbeirat (scientific advisory board Meeting) of the Max Planck Institute for the Structure and Dynamics of Matter
Hamburg (Germany), 9 – 11 march 2016

Towards ab-initio molecular dynamics without Born-Oppenheimer potential-energy surfaces (oral communication)
G. Albareda, A. Abedi, I. Tavernelli, A. Rubio

Fotofuel – Summer School
Almeria (Spain), 25 – 27 october 2016

Theoretical modelling of light harvesting materials (oral communication)
F. Viñes

Festival of Genomics
London (UK), 19 – 21 january 2016

Chemical basis for the recognition of trimethyllysine by epigenetic reader proteins (poster)
J. Poater, F. M. Bickelhaupt, J. Mecinovic

funCOS
Erlangen (Germany), 29 july 2016

Theoretical modelling of catalytic materials and their reactivity: as simple as possible, but not simpler (invited talk)
K. M. Neyman

115th General Assembly of the German Bunsen Society for Physical Chemistry, Bunsentagung 2016
Rostock (Germany), 5 -7 may 2016

Low platinum group metal fuel cell catalysts: from surface science to in-situ spectroelectrochemistry (oral communication)
O. Brummel, F. Waidhas, F. Faisal, M. Vorokhta, I. Khalakhan, G. Kovács, S. Kozlov, K. M. Neyman, V. Matolin, J. Libuda.

General Assembly meeting of the FP7 project ChipCAT Design of Thin-Film Nanocatalysts for On-Chip Fuel Cell Technology
Prague (Czech Republic), 9 – 10 may 2016

Progress report on the work package 2 "Computational modelling" (oral communication)
K. M. Neyman

General Meeting of the COST Action CM1104 Reducible oxide chemistry, structure and functions
Osnabrück (Germany), 6 – 8 april 2016

Modeling interactions of transition metals with ceria nanoparticles: applications for fuel cell technologies (poster)
A. Figueroba, K. M. Neyman

Modelling of ceria-based nanostructured inspired by the action CM1104 (oral communication)
K. M. Neyman, A. Figueroba, S. M. Kozlov

Metal-oxide interactions in Pt/CeO_2 catalysts and related phenomena (oral communication)
Y. Lykhach, S. M. Kozlov, A. Bruix, G. N. Vayssilov, T. Skála, A. Tovt, N. Tsud, V. Stetsovych, F. Dvo□ák, V. Johánek, A. Neitzel, J. Myslivecek, I. Matolínová, M. Vorokhta, K. Ševcíková, R. Fiala, M. Václavu, K. C. Prince, S. Bruyère, V. Potin, A. Migani, T. Staudt, G.P. Petrova, F. Illas, S. Fabris, V. Matolín, K.M. Neyman, J. Libuda

12th German Conference on Chemoinformatics
Fulda (Germany), 6 -8 november 2016

The "NOMAD (novel materials discovery) center of excellence": challenges and solutions to build a code-independent data base for computational materials science and its implication in computational chemistry (oral communication)
F. Illas

Girona Seminar. Predictive catalysis: Transition-metal reactivity by design
Girona (Spain), 17 – 20 april 2016

Electronic structure and reactivity of donor-stabilized bis(amididinato/guanidinato) silylenes (poster)
J. Poater, C. F. Guerra, F. M. Bickelhaupt, R. Tacke

High Dimensional Quantum Dynamics – challenges and opportunities
Rostok (Germany), 31 august – 3 september 2016

Diabatization of the H_2@SWNT system within the MCTDH approach: circumventing potential energy matrix calculations (oral communication)
M. Mondelo-Martell, F. Huarte-Larrañaga

HPC Materials Chemistry Consortium
Cardiff (UK), 16 november 2016

From building blocks to bulk: design and understanding of nanostructured materials from the bottom-up (oral communication)
S. T. Bromley

Interfaces Against Pollution - IAP2016
Lleida (Spain), 4 – 7 september 2016

Functionalized surfaces with tailored wettability determine influenza A infectivity (poster)
I. Mannelli, R. Reigada

One century of the Langmuir adsorption isotherm (poster)
F. Mas, C. Rey-Castro

Dealing with electrostatic interctions in the determination of ion binding properties of polyelectrolytes. Extension of the transfer matrix formalism to the full range of ionic strengths (poster)
J.L. Garcés, S. Madurga, C. Rey-Castro, F. Mas

F. Mas *(organizing committee)*

42nd International Conference on Coordination Chemistry
Brest (France), 3 – 8 july 2016

Transport properties of single-molecule devices showing room temperature magnetoresistance (invited talk)
E. Ruiz

Computational modeling of the ligand tuning effect over the transition temperature in spin-crossover systems (oral communication)
J. Cirera, E. Ruiz

Disentangling a long lasting issue: which is the magnetic dimensionality of the Cu_2(1,4-diazacycloheptane)$_2Cl_4$ crystal? (oral communication)
J. Jornet-Somoza, F. Cosi, M. Fumanal, M. Deumal

X International Conference on Mechanisms of Catalytic Reactions, School-Symposium on Quantum-mechanical modelling of catalytic processes
Svetlogorsk (Russia), 2 – 6 october 2016

Innovative computational design of advanced nanoalloy materials for catalysis and beyond (invited talk)
K. M. Neyman

K. M. Neyman (*chairman*)

8th International Conference on Molecular Electronics - ElecMol 2016
Paris (France), 22 – 26 august 2016

New fundamental effects in single-molecule circuitry (oral communication)
A. C. Aragonès, N. Darwish, F. Sanz, I. Díez-Pérez

15th International Conference on Molecule-Based Magnets - ICMM2016
Sendai (Japan), 4 – 8 september 2016

On the mechanism of bistability in three dithiazolyl molecule-based magnetic crystals (poster)
T. Francese, M. Deumal, J. Ribas-Ariño, J. J. Novoa

Magnetoresistance at room temperature in single-molecule porphyrin-based devices (oral communication)
E. Ruiz

16th International Conference on Theoretical Aspects of Catalysis - ICTAC-16
Zakopane (Poland), 19 – 23 june 2016

Transition metal carbides based catalysts for CO_2 conversion: computational modeling and experiments (invited talk)
S. Posada-Perez, F. Viñes, J. A. Rodriguez, P. Liu, D. J. Stacchiola, P. J. Ramírez, R. A. Gutiérrez, F. Illas

Computationally designed nanoparticle as advanced models of bimetallic catalysts (invited talk)
K. M. Neyman

K. M. Neyman (*chairman*)

16th International Congress on Catalysis – ICC 2016
Beijing (China), 3 – 8 july 2016

Metal-carbide synergism in heterogeneous catalysis: an overview (oral communication)
F. Viñes, P. Liu, J. A. Rodriguez, F. Illas

Efficient in-silico design of advanced nanoalloy materials for catalysis and related applications (invited talk)
K. M. Neyman, G. Kovács, S. M. Kozlov

International Focus Workshop on Bridging-Time Scale Techniques and their Applications in Atomistic Computational Science
Dresden (Germany), 12 – 15 september 2016

The variational nature of some reaction path models (oral communication)
J. M. Bofill, W. Quapp

The use of Newton trajectories in mechanochemistry and catalysis (oral communication)
W. Quapp, J. M. Bofill

18th International Symposium on Small Particles and Inorganic Clusters - ISSPIC
Jyväskylä (Finland), 14 – 19 august 2016

Computational engineering of bimetallic nanocrystals with tailor-made atomic ordering (oral communication)
S. M. Kozlov, K. M. Neyman, G. Kovács, Z. Cao, L. Falivene, L. Cavallo

International Symposium on Single-Atom Catalysts
Dalian (China), 30 june – 2 july 2016

Materials for single-atom catalysis based on nanostructured ceria: Density-functional modelling (invited talk)
K. M. Neyman

K. M. Neyman (*chairman*)

7th IQTCUB Symposium
Barcelona (Spain), 10 june 2016

Single molecule motors working on surface (invited talk)
J. Echeverría

Adsorption and separation of post-combustion gases with Mg-MOF-74 (poster)
F. Keshavarz, X. Giménez, D. Bahamón, P. Gamallo, R. Sayós

Nomad, the novel materials discovery laboratory (invited talk)
R. Valero, A. H. Larsen, S. T. Bromley, F. Illas

Using open-shell molecules to design 2D covalent networks with controllable properties (poster)
I. Alcón, S. T. Bromley, F. Illas

Selective capture and separation of industrial post-combustion gases with FAU-type zeolites: a computational study (poster)
H. Prats, G. Alonso, D. Bahamón, X. Giménez, P. Gamallo, R. Sayós

Stability of ZnO nanoparticles as function of shape and size (poster)
O. Lamiel-Garcia, F. Viñes, F. Illas, S. T. Bromley

Performance of density functional theory based methods in predicting core level binding energies and the physical meaning of Khon-Sham energies (poster)
N. Pueyo-Bellafont, P. S. Bagus, F. Illas

Highly active Cu/β-Mo_2C and Cu/δ-MoC catalysts for the conversion of CO_2: The metal/C ratio as a key factor defining activity, selectivity, and stability (poster)
S. Posada-Pérez, P. J. Ramírez, J. Evans, F. Viñes, P. Liu, F. Illas, J. A. Rodriguez

Graphene interaction with Ni(111) descripted by modern dispersive forces (poster)
H. Muñoz-Galán, F. Viñes, J. Gebhardt, A. Görling, F. Illas

A conditional wave function approach to reactive scattering (poster)
E. Bernuz, J. M. Bofill, F. Illas, G. Albareda

Extension of the transfer matrix methods to include long-range interactions (poster)
J. L. Garcés, P. M. Blanco, S. Madurga, F. Mas

Brownian dynamics simulations of enzymatic reaction-diffusion processes in crowded intracellular environments (poster)
M. Via, P. M. Blanco, S. Madurga, J. L. Garcés, F. Mas

Macromolecular crowding effect on the cooperativity of enzymatic reactions (poster)
N. Vilaplana, C. Balcells, S. Madurga, J. L. Garcés, M. Cascante, F. Mas

Jornada catalana de supercomputació – recerca i supercomputació: compartint memòries i avançant el futur
Barcelona (Spain), 25 may 2016

Simulacions computacionals per a entendre com funcionen els enzims (oral communication)
C. Rovira

Master Química XII
Barcelona (Spain), 18 may 2016

Simulació per Dinàmica Browniana de processos de difusió de proteïnes en medis intracel·lulars (poster)
P. M. Blanco, M. Via, S. Madurga, F. Mas

Efecte de l'aglomeració macromolecular sobre la cooperativitat de l'enzim glutamat-deshidrogenasa (poster)
N. Vilaplana, C. Balcells, S. Madurga, J. L. Garcés, M. Cascante, F. Mas

NOMAD PI & SAC Meeting
Barcelona (Spain), 3 – 5 october 2016

CO_2 Adsorption and Activation: Identifying Materials and Descriptors (oral communication)
C. Kunkel

***Not Strictly Inorganic Chemistry* - NOSIC-7**
Prullans (Spain), 1 – 3 june 2016

Kurt Vonnegut's cat's cradle: a tale on science, religion and human stupidity (oral communication)
P. Alemany

Olivier Kahn Discussions
Bordeaux (France), 26 – 28 may 2016

Molecular Mechanisms of Spin Crossover in the {Fe(pz)[Pt(CN)$_4$]} Metal-Organic Framework upon Water Adsorption (oral communication and poster)
J. Cirera, F. Paesani

Partnership for advanced computing in Europe - PRACEdays16
Prague (Czech Republic), 10 – 12 may 2016

Computer simulation to understand how enzymes work (oral communication)
C. Rovira

6th Phase Transition and Dynamical properties of Spin Transition Materials
Gandia (Spain), 27 – 30 november 2016

Spin crossover systems: from quantum transport to microporous materials *(invited talk)*
E. Ruiz

Quantum Dynamics: from Algorithms to Applications
Greifswald (Germany), 5 – 8 september 2016

Diabatization of the H_2@SWNT system within the MCTDH approach: time scale separation of confined and free coordinates (oral communication)
M. Mondelo-Martell, F. Huarte-Larrañaga

Reducible oxide chemistry, structure and functions COST Action CM1104, Final General meeting
Osnabrück (Germany), 6 – 8 april 2016

Towards a first principles description of realistic models of TiO_2 nanoparticles (oral communication)
O. Lamiel-García, K. C. Ko, S. T. Bromley, J. Y. Lee, F. Illas

XXXII Reunió de la xarxa de Referència en Química Teòrica i Computacional de Catalunya - XrQTC
Barcelona (Spain), 4 – 5 july 2016

On the mechanism of bistability in molecule-based magnets (oral communication)
T. Francese, M. Deumal, J. Ribas-Ariño, J. J. Novoa

Computational study of the Si/Al ratio effect in FAU-type zeolites for CO_2 post-combustion capture (oral communication)
D. Bahamón, H. Prats, P. Gamallo, G. Alonso, X. Giménez, R. Sayós

Density functional theory description of the electronic structure of realistic models of TiO_2 nanoparticles (oral communication)
O. Lamiel-Garcia, K. C. Ko, S. T. Bromley, F. Illas

Mo carbides for the conversion of CO_2: the metal/C ratio as a key factor (oral communication)
S. Posada-Pérez, P. J. Ramírez, J. Evans, F. Viñes, P. Liu, F. Illas, J. A. Rodriguez

Using open-shell molecules to design 2D covalent networks with controllable properties (oral communication)
I. Alcón, F. Illas, S.T. Bromley

Conditional Born-Oppenheimer dynamics (oral communication)
E. Bernuz, J. M. Bofill, F. Illas, G. Albareda

Towards ab-initio molecular dynamics without Born-Oppenheimer potential-energy surfaces (oral communication)
G. Albareda

Molecular sieving of H_2 and D_2 in a carbon nanotube: kinetic vs thermodynamic effects (oral communication)
M. Mondelo-Martell, F. Huarte-Larrañaga

Prebiotic Reactions base on Titan's Atmosphere Chemistry (oral communication)
E. López, D. Ascenzi, P. Tosi, J. M. Bofill, A. Aguilar

Effect of mixed crowded media on the diffusion processes of proteins in intracellular media by Brownian dynamics simulations (oral communication)
P. M. Blanco, M. Via, S. Madurga, J. L. Garcés, F. Mas

III Reunión de Jóvenes Investigadores en Coloides e Interfases - JICI
Madrid (Spain), 13 – 14 october 2016

Risk assessment of manufactured nanomaterials. Where classical theories of Colloids and Interfaces meet emerging environmental challenges in the 21st Century (invited talk)
C. Rey-Castro, C. David, F. Mas, J. Galceran, J. Puy

Brownian dynamics of the macromolecular crowding effect in reaction-diffusion process in cellular media (oral communication)
P. M. Blanco, M. Via, S. Madurga, J. L. Garcés, E. Vilaseca, F. Mas

Seminar at Instituto de Física de la Materia Condensada (IFIMAC) 2016
Madrid (Spain), 2 june 2016

Exploring external stimuli to modulate the conductance in single-molecule wires at room conditions (invited talk)
I. Díez-Pérez

Seminar at Jagiellonian University
Krakow (Poland), 17 june 2016

Theoretical modelling of catalytic materials: as simple as possible, but not simpler (invited talk)
K. M. Neyman

Seminar at Université de Bretagne Occidentale (UMR CNRS 6521)
Brest (France), 1 july 2016

Computational Modeling of the ligand tuning effect over the transition temperature in Spin-Crossover systems (invited talk)
J. Cirera

XXV Sitges Conference on Statistical Physics. Nonequilibrium Phenomena in Confined Systems
Barcelona (Spain), 6 – 10 june 2016

Effect of mixed crowded media on the diffusion processes of proteins in intracellular media by Brownian dynamics simulations (invited talk)
P. M. Blanco, M. Via, S. Madurga, J. L. Garcés, F. Mas

Extension of the transfer matrix methods to include long-range interactions in polyelectrolytes (poster)
J. L. Garcés, P. M. Blanco, S. Madurga, F. Mas

Macromolecular crowding effect on the cooperativity of enzymatic reactions (poster)
N. Vilaplana, C. Balcells, S. Madurga, J. L. Garcés, M. Cascante, F. Mas

VI Simpósio de Estrutura Eletrônica e Dinâmica Molecular - SeedMol 2016
Alto Paraíso de Goiás (Brasil), 19 – 23 september 2016

Metal-carbide synergism in heterogeneous catalysis: an overview (invited talk)
F. Viñes, P. Liu, J. A. Rodriguez, F. Illas

XIII Simposio de Investigadores Jóvenes de la RSEQ
Logroño (Spain), 8 – 11 november 2016

Simulaciones computacionales en procesos de elevado interés industrial (invited talk)
P. Gamallo, H. Prats, G. Alonso, X. Giménez, D. Bahamón, R. Sayós

III Simposio de Jóvenes Investigadores de la SEQT
Barcelona (Spain), 17 june 2016

Synthesis and biological activity of new resveratrol derivatives (poster)
L. Grau, R. Soucek, J. Rubio, M. D. Pujol

State of the art in bistable magnetic molecules - post-ICMM Symposium
Fukuoka (Japan), 10 september 2016

First-principles theoretical studies on the mechanism of bistability in molecule-based magnets: the PDTA case (oral communication)
T. Francese, M. Deumal, J. Ribas-Ariño, J. J. Novoa

1st Symposium of the Research Unit NAGOCAT – Nanoporous Gold Catalysts - FOR2213
Delmenhorst (Germany), 8 – 9 september 2016

Progress in modelling of catalytic materials: engineering of bimetallic nanocrystallites (invited talk)
K. M. Neyman

Symposium on Size-Selected Clusters 2016
Davos (Switzerland), 28 february – 4 march 2016

Size dependent greenness: bottom-up versus top-down approaches to understanding titania clusters (oral communication)
S. T. Bromley

52nd Symposium on Theoretical Chemistry - STC 2016
Bochum (Germany), 26 – 29 september 2016

The key role of second order phase transitions in dithiazolyl-based switchable magnetic materials (poster)
S. Vela, M. Deumal, J. J. Novoa, J. Ribas-Ariño

Telluride Science Research Center 2016 Workshop
Telluride (USA), 26 june – 2 july 2016

Spin dependent transport in single-molecule wires at room temperature (invited talk)
I. Díez-Pérez, A. C. Aragonès, M. Ferrer, N. Gimeno, M. Teixidor, E. Giralt, V. Mujica

17th Tetrahedron Symposium - Challenges in Biological, Bioorganic & Medicinal Chemistry
Sitges (Spain), 28 june – 1 july 2016

Synthesis of 2,6-bis(benzyliden)piperidin-4-one with potential antitumor activity (poster)
L. Navarro, J. Rubio, M. D. Pujol

Design and synthesis of arylamides as potential G6PDH inhibitors (poster)
L. Acedo, J. Rubio, M. D. Pujol

The Osaka City University International Conference on Molecular Spins and Quantum Technology - OCUIC-2016
Osaka (Japan), 31 august – 4 september 2016

The mechanism of bistability in three dithiazolyl molecule-based magnetic crystals (invited talk)
J. J. Novoa, J. Ribas-Ariño, T. Francese, S. Vela, M. Deumal.

On the mechanism of bistability in prototype PDTA molecule-based magnets (oral communication)
T. Francese, M. Deumal, J. Ribas-Ariño, J. J. Novoa

Theoretical Challenges: Simulating Materials out of Equilibrium
Hamburg (Germany), 1 – 3 june 2016

Towards ab-initio molecular dynamics without Born-Oppenheimer potential-energy surfaces (invited talk)
G. Albareda, A. Abedi, I. Tavernelli, A. Rubio

Theoretical Modelling of Nanoparticulate Materials: Theory Catching up with Experiment
Barcelona (Spain), 30 september 2016

Graphene interaction with Ni(111) descripted by modern dispersive forces
H. Muñoz-Galán, F. Viñes, J. Gebhardt, A. Görling, F. Illas

Bcc transition metal surfaces: trends in work functions and surface energies
L. Vega, F. Viñes

Mo carbides for the conversion of CO_2: the metal/C ratio as a key factor
S. Posada-Pérez, P. J. Ramírez, J. Evans, F. Viñes, P. Liu, F. Illas, J. A. Rodriguez

A. Figueroba, G. Kovács *(meeting organizers)*

K. M. Neyman *(chairman)*

9ª Trobada de Joves Investigadors dels Països Catalans
Perpignan (France), 3 – 5 february 2016

Selective capture and separation of industrial post-combustion gases using different zeolites. A theoretical approach (oral communication)
G. Alonso, F. Keshavarz, H. Prats, P. Gamallo, X. Giménez, R. Sayós

Difusió en medis intracel·lulars. Simulació per dinàmica browniana (oral communication)
M. Via, P. M. Blanco, S. Madurga, F. Mas

R. Sayós *(meeting organizing committee)*

4th TYC Energy Materials Workshop: Shaping Nanocatalysts
London (UK), 14 – 16 december 2016

Modeling realistic TiO_2 nanoparticles for improved photocatalytic activity from density functional theory based calculations (invited talk)
F. Illas

Sophisticated computational design of bimetallic nanocrystallites (invited talk)
K. M. Neyman, G. Kovács, S. M. Kozlov

K. M. Neyman (*chairman*)

Workshop on Advanced Functional Materials
Pravets (Bulgaria), 14 – 16 october 2016

Computational modelling of inorganic nanomaterials for catalysis and energy technologies (invited talk)
K. M. Neyman

RESEARCH STAYS IN RECOGNIZED CENTERS

Albareda, G.	**Max Planck Institute for the Structure and Dynamics of Matter**, **Hamburg (Germany)** UB visiting researcher invited by A. Rubio. March and November 2016
Albertí, M.	**Univeristà di Perugia, Perugia (Italy)** Research stay. Dipartimento di Chimica, Biologia e Biotecnologie. February-July 2016
Alemany, P.	**Departamento de Química, Universidad Católica del Norte, Antofagasta (Chile)** Research stay. October 2016
Alemany, P.	**Department of Materials Science and Engineering, Kyoto University, Kyoto (Japan)** Research stay. July 2016
Climent, C.	**Donostia International Physics Center, Donostia (Spain)** PhD stay. July 2016
Climent, C.	**Institut de Chimie Radicalaire, Marseille (France)** PhD stay. September-November 2016
Díez-Pérez, I.	**Weizmann Institute of Science**, **Rehovot (Israel)** UB visiting researcher invited by Ron Naaman. December 2016
López, M.	**Laboratoire d'Electrochimie Moléculaire**, **UMR CNRS, Université Paris 7, Paris (France)** PhD stay with Christophe Demaille. October-December 2016
Neyman, K. M.	**Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen (Germany)** Invited visiting researcher. July-August 2016
Neyman, K. M.	**Uppsala University, Uppsala (Sweden)** Invited visiting professor. December 2016
Poater, J.	**Vrije Unvirsiteit Amsterdam (The Netherlands)** UB visiting researcher invited by F. M. Bickelhaupt. March-June 2016
Reigada, R.	**Max Planck Institute, Berlin (Germany)** Invited Professor invited by A. Mikhailov, Complex Systems Group. May 2016

PARTICIPATION IN COMPETITIVE FUNDED RESEARCH PROJECTS

Xarxa de Referència d'R+D+I en Química Teòrica i Computacional (XRQTC)
Francesc Illas Riera, Universitat de Barcelona
2014
Departament d'Innovació, Universitats i Empresa. Generalitat de Catalunya

Grup de Dinàmica de Reaccions Químiques
Antonio Aguilar Navarro, Universitat de Barcelona
2014SGR0025, 2014-2016
Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR)

Grup de Recerca Reconegut i Finançat per la Generalitat de Catalunya
Francesc Illas Riera
Universitat de Barcelona
2014SGR97, 2014-2016
Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR), Generalitat de Catalunya

Química Orgànica Experimental, Teòrica i Computacional
Josep Maria Bofill Vilà, Universitat de Barcelona
2014SGR139, 2014-2016
Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR)

Grup d'Estructura Electrònica.
Santiago Alvarez Reverter, Universitat de Barcelona
2014SGR662, 2014-2016
Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR)

Grup d'Estructura i funció en macromolècules
Carme Rovira Virgili, Universitat de Barcelona
2014SGR987, 2014-2016
Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR)

Grup de Bioquímica Integrativa
Marta Cascante Serratosa, Universitat de Barcelona
2014SGR1017, 2014-2016
Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR)

Grup Nanoprobes
Ismael Díez-Pérez, Pau Gorostiza i Fausto Sanz, Universitat de Barcelona & IBEC
2014SGR1251, 2014-2016
Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR)

Simulació molecular aplicada (MOLSIMAP)
Fèlix Lluís Llovell Ferret, IQS, Universitat Ramon Llull
2014SGR1582, 2014-2016
Grup de Recerca Reconegut i Finançat per la Generalitat de Catalunya
Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR)

ICREA Acadèmia
Francesc Illas, Universitat de Barcelona
2016-2020
Institut Català de Recerca Avançada (ICREA, Generalitat de Catalunya)

ICREA Acadèmia
Eliseo Ruiz, Universitat de Barcelona
2014-2018
Institut Català de Recerca Avançada (ICREA, Generalitat de Catalunya)

Beca Postdoctoral Beatriu de Pinos.
Jordi Cirera, Universitat de Barcelona
2014-2016
AGAUR (Generalitat de Catalunya)

Beca Postdoctoral Juan de la Cierva.
Jorge Echeverría, Universitat de Barcelona
2016-2018
Ministerio de Economía y Competitividad

Structure and surface composition of Pt-based bimetallic nanoparticles for catalysis and beyond
Konstantin Neyman, Universitat de Barcelona
QCM-2016-2-0020, QCM-2016-3-0015, 2016-2017
Red Española de Supercomputación (RES)

Structure and surface composition of Ni-based bimetallic nanoparticles as catalysts
Konstantin Neyman, Universitat de Barcelona
QCM-2015-3-0012, QCM-2016-1-0006, 2015-2016
Red Española de Supercomputación (RES)

Diseño computacional de pares de bases de ADN artificiales que pueden ser replicados.
Jordi Poater, Universitat de Barcelona
CTQ2016-77558-R, 2017-2019
Ministerio de Economía y Competitividad (MINECO)

Estudio Computacional del Control Mecanoquímico de Reacciones de Interés en Química Biorgánica.
Josep Maria Bofill Villà & Ibério de P. R. Moreira, Universitat de Barcelona
CTQ2016-76423-P, 2017-2019
Ministerio de Economía y Competitividad (MINECO)

Plugging Biomolecules on surfaces.
Ismael Díez-Pérez, Universitat de Barcelona
CTQ2015-71406-ERC, 2015-2016
Ministerio de Economía y Competitividad (MINECO)

Comprension, Control y Optimizacion en Catalisis Heterogenea y Fotocatalisis en la Nanoescala. Aplicacion a la Conversion De Dioxido De Carbono y a la Produccion de Hidrogeno
Francesc Illas Riera i Stefan T. Bromley, Universitat de Barcelona
CTQ2015-64618-R, 2016-2018
Ministerio de Economia y Competitividad (MINECO)

Estructura electrónica y propiedades en moléculas y sólidos.
Eliseo Ruiz Sabín, Universitat de Barcelona
CTQ2015-64579-C3-1-P, 2016-2018
Ministerio de Economía y Competitividad

Estructura electrónica y propiedades de moléculas y sólidos.
Pere Alemany Cahner i Ismael Díez-Pérez, Universitat de Barcelona
CTQ2015-64579-C3-3-P, 2016-2018
Ministerio de Economia y Competitividad (MINECO)

Moduladores fotoconmutables sintéticos para manipular remotamente proteínas endógenas: fotocontrol in vivo de canales iónicos pentaméricos.
Carme Rovira Virgili, Universitat de Barcelona
PCIN-2015-163-C02-01, 2015-2017
Ministerio de Economia y Competitividad (MINECO)

Captura y separación de gases y contaminantes en procesos Industriales sostenibles
Ramón Sayós Ortega i Pablo Gamallo Belmonte, Universitat de Barcelona
CTQ2014-53987-R, 2015-2017
Proyectos I+D+I del programa estatal de investigación, desarrollo e innovación orientada a los retos de la Sociedad
Ministerio de Economia y Competitividad (MINECO)

Simulation of reactive processes in proteins and enzymes by means of ab initio molecular dynamics and QM/MM techniques.
Carme Rovira Virgili, Universitat de Barcelona
CTQ2014-55174-P, 2015-2017
Ministerio de Economia y Competitividad (MINECO)

FOTOFUEL – New Challenges in the Production of Solar Fuels
Francesc Illas *Riera,* Universitat de Barcelona
ENE2014-52280 -REDT, 2013-2016
Ministerio de Economia y Competitividad (MINECO)

Mecanismo de transición de fase e interacción magnética en cristales moleculares magnéticos que presentan transición de espín
Mercè Deumal i Juan J. Novoa Vide, Universitat de Barcelona
MAT2014-54025-P, 2015-2017
Ministerio de Economia y Competitividad (MINECO)

Experimentación y modelización computacional de dinámica de reacciones químicas.
Antonio Aguilar Navarro i Fermín Huarte Larrañaga, Universitat de Barcelona
CTQ2013-41307-P, **2014-2016, prorrogat 2017**
Ministerio de Economía y Competitividad (MINECO)

Materia blanda forzada, activa y viva.
Jaume Casademunt Viader i Francesc Sagués Mestre, Universitat de Barcelona
FIS2013-41144P, 2014-2016
Ministerio de Economia y Competitividad (MINECO)

Knowledge Led Structure Prediction for Nanostructures
Scott Woodley, University College London
EP/K038958/1, 2013-2018
Engineering and Physical Sciences Research Council (UK)

Computational modelling and molecular dynamics simulations of oil/water wettability on carbonate rocks and clays
Ramón Sayós Ortega / Pablo Gamallo Belmonte, Universitat de Barcelona
Referència **308465**
Contracto de arrendamientos y servicios de I+D con REPSOL, S.A.

COMPHOTOCAT: - Computational design of TiO_2 based nanoparticles for improved photocatalytic activity towards water splitting under visible sunlight
Francesc Illas Riera
Universitat de Barcelona
PRACE - 2014112608, 2015-2016
Partnership for Advanced Computing in Europe (PRACE)

Reducible oxide chemistry, structure and functions
Michael Reichling, Universität Osnabrück
Francesc Illas Riera, (representative of Spain), Konstantin Neyman (deputy representative of Spain),
Universitat de Barcelona
CM1104, 2012-2016
European Framework for Cooperation in Science and Technology (COST)

Explicit Control Over Spin-States in Technology and Biochemistry
Marcel Swart (University of Girona), Carme Sousa Romero (participant of the Universitat of Barcelona)
Universitat de Barcelona
CM1305, 2014-2018
European Framework for Cooperation in Science and Technology (COST)

Materials Networking
Konstantin Neyman, Universitat de Barcelona
European Commission, Ref. Nº 692146, 2016-2019
European H2020 Cooperation Program - Research theme: 'Twinning' (H2020)

Design of thin-film nanocatalysts for on-chip fuel cell technology
Konstantin Neyman, Universitat de Barcelona
FP7-NMP.2012.1.1-1, Ref. No.310191, 2012-2016
European FP7 'Cooperation' - Research theme: 'Nanosciences, nanotechnologies, materials and new production technologies'

Theoretical Chemistry and Computational Modelling
Juan Novoa Vide, Universitat de Barcelona
H2020-MSCA-ITN-2014-642294
H2020, Innovative Training Networks

Theoretical Chemistry and Computational Modelling
Manuel Yanez, Universidad Autonoma de Madrid
TCCM-EJD, 2014-2018
H2020 – ITN, Research and Innovation Framework Programme

A comprehensive and standardised e-infrastructure for analysing medical metabolic phenotype data (PhenoMeNal)
Marta Cascante Serratosa
8P1ERI - H2020. PILLAR 1-EXCELLENT SCIENCE. ERI. European Research Infrastructures, 2015-2018.
Unió Europea.

Theoretical Chemistry and Computational Modelling (TCCM)
Juan Jose Novoa Vide
8P1MCA - H2020 PILLAR 1-EXCELLENT SCIENCE. MCA. Marie Sklodowska-Curie Actions, 2015-2018.
Unió Europea.

Deciphering the Metabolism of Haematological Cancers (HaemMetabolome)
Marta Cascante Serratosa
8P1MCA - H2020. PILLAR 1-EXCELLENT SCIENCE. MCA. Marie Sklodowska-Curie Actions, 2015-2018
Unió Europea.

Enhancing the scientific capacity of the Faculty of Chemistry and Pharmacy at Sofia University as leading regional research and innovation centre in the area of advanced functional materials (Materials Networking)
Konstantin Neyman
8SEWP - H2020. SEWP. Spreading Excellence and Widening Participation, 2016-2019
Unió Europea.

QUIFIEXP - Química Física Experimental
Jordi Ignes Mullol
GINDO-UB/112, 2016-2019
PPID - Projectes d'Innovació Docent (UB)

NOMAD – Novel Materials Discovery
Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin
NoMaD - 676580, 2015-2018
H2020-EINFRA-5-2015, Centers of Excellence for Computing Applications

Synthesis, characterization, and optical properties of $LN_{2-X}RE_XWO_6$ (LN=Y^{3+}); RE= Dy^{3+}, Er^{3+}, Eu^{3+}, Sm^{3+} and Yb^{3+}) downconversion luminiscent materials and their application in dye sensitized solar cells.
Jaime Llanos, Universidad Católica del Norte, Antofagasta (Xile)
Fondecyt Regular nº 1130248, 2013-2016
Comisión Nacional de Investigación Científica y Tecnológica (CONICYT, Xile)

Reducible oxide chemistry, structure and functions
Konstantin Neyman, Universitat de Barcelona (deputy Spanish representative in the Management Committee)
CM1104, 2012-2016
European Framework for Cooperation in Science and Technology (COST)

Single-Molecule studies of photo-conductance on photosynthetic molecular systems by SPM break-junction measurements.
Ismael Díez-Pérez, Pau Gorostiza, Universitat de Barcelona & IBEC
FP7-277182, 2012-2016
FP7-EU

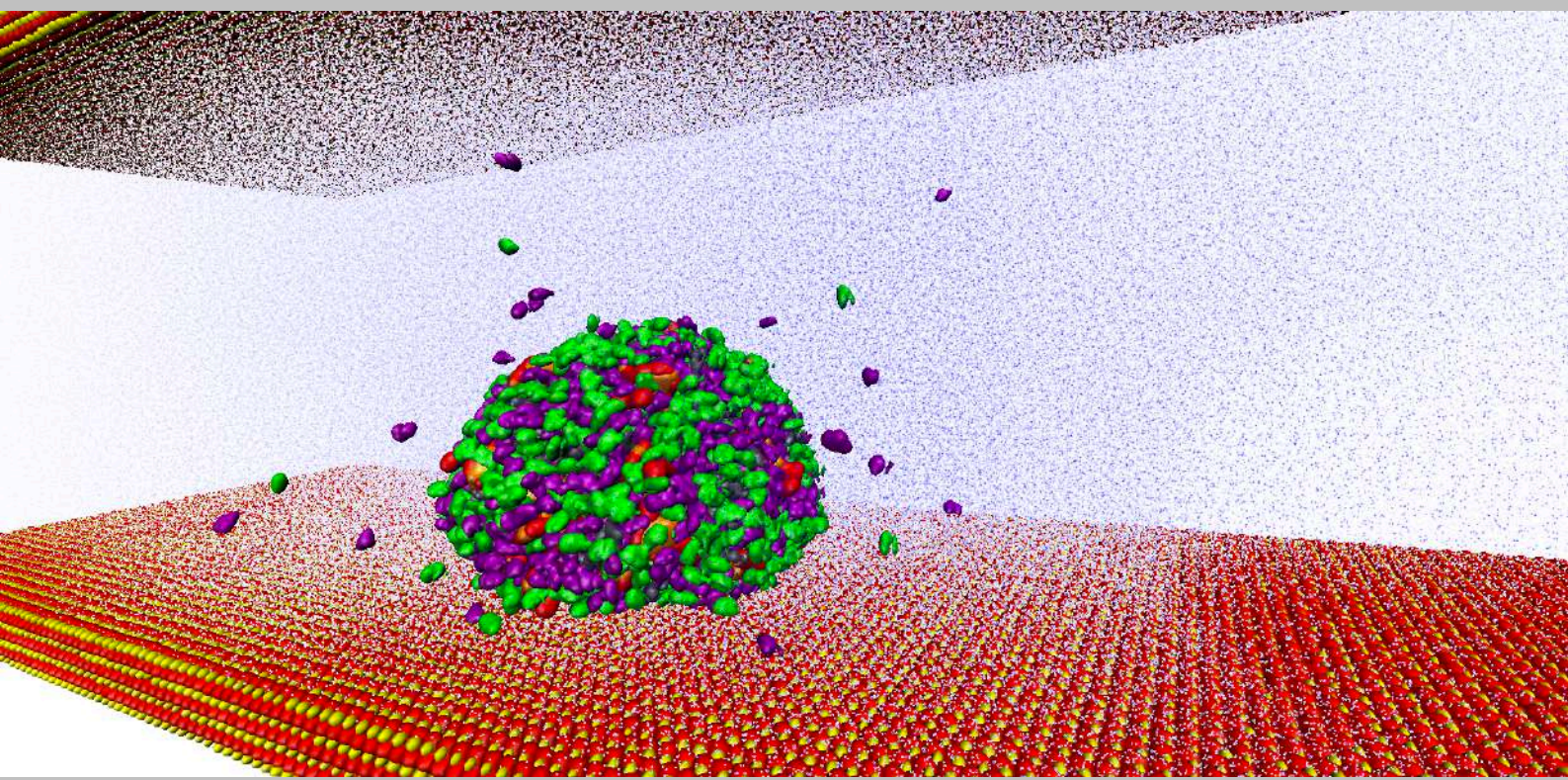
Developing single-molecule switches for applications in nanoscale organic devices (Single-Molec-Switch).
Ismael Díez-Pérez, Nadim Darwish, Universitat de Barcelona
PIIF-GA-2012-328893, 2013-2016
FP7-EU

Molecularly Assembled Electrodes.
Jorge Pavez, Ismael Díez-Pérez (as International partner), Universitat de Santiago de Chile, Universitat de Barcelona
Fondecyt, 2013-2017
FONDECYT

Institut de Química Teòrica
i Computacional
UNIVERSITAT DE BARCELONA

UNIVERSITAT DE BARCELONA

Institut de Química Teòrica i Computacional de la Universitat de Barcelona (IQTCUB)



Activity Report 2016