Institut de Química Teòrica
i Computacional
UNIVERSITAT DE BARCELONA

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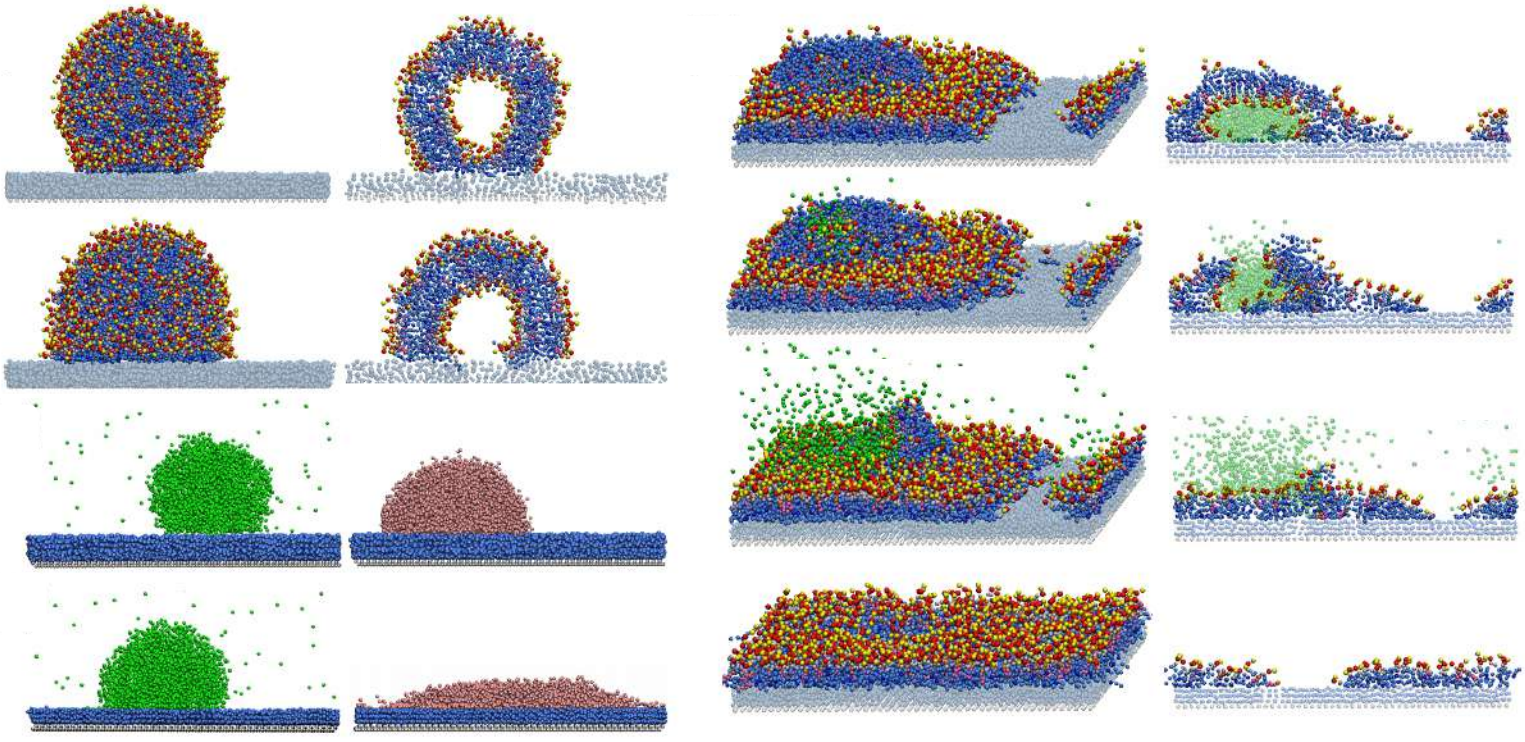
Institut de Química Teòrica i Computacional de la Universitat de Barcelona (IQTCUB)



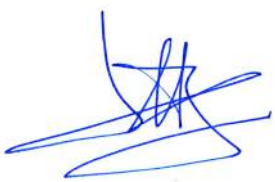
Activity Report 2017

This memory is dedicated to Professor Jaime de Andrés Llopis (1946-2017),
who passed away unexpectedly on September 13th, 2017.

His inspiring positivism and global erudition will remain unforgotten.

The creation of the Institute of Theoretical Chemistry of the *Universitat de Barcelona* (IQTCUB) was approved on November 27th, 2007. From that quite far away date I have had the honour to serve as Director, a duty I tried to carry out in spite of the many difficulties arising from the strong economical crisis that has bitten us all over during this time. After two formal terms as director, and overseeing the running of the institute for a long period between elections, the mandatory and necessary change in leadership must proceed. I would like to take the opportunity of writing the preface of this year's IQTCUB memoir to explicitly thank Drs. Ramón Sayós and Carme Rovira Virgili for their constant support as members of the director team, Drs. Pere Alemany and Josep Maria Bofill for having served as the first IQTCUB director team, the IQTCUB group leaders to believe in this project that, step-by-step, has been fully consolidated and, not forgetting, the constant support from the various Rector teams of the Universitat de Barcelona. No less important has been the support from our technical staff members Teresa Arenal and Jordi Inglés who, with a dedication of almost 24 hour a day and 7 days a week, in conditions that one may describe as far from optimal, have maintained the computing system efficiently working, notwithstanding to numerous power cuts and frequent temperature rises which endanger the whole system.

I would like to end by recalling that 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 Modelling), a research field not involving a typical chemical laboratory but rather a virtual "computational laboratory" with supercomputers having hundreds or thousands of processors. Research at 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 often cannot be obtained with other methods. Therefore, the tools developed and employed in the IQTCUB play a prime role in helping to solve many of the pressing challenges faced by modern society. The IQTCUB is over ten years old and this year's *activity report* demonstrates its ongoing and increasing vitality and growth through considerable scientific production in research lines as diverse as drug design, heterogeneous catalysis, nanostructures, novel materials, and atmospheric chemistry, clearly showing the high impact of our research. The continuation of the IQTCUB's success and its enhancement in the future is a goal that, no doubt, will be achieved by the new directorship team and one for which they will have all my support and enthusiasm.



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 90 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)

Cirera Fernández	Jordi	Inorganic and Organic Chemistry	Inorganic Chemistry
Figueras Valls	Marc	Materials Science & Physical Chemistry	Physical Chemistry
Jover Modrego	Jesús	Inorganic and Organic Chemistry	Inorganic Chemistry
Martínez-Alanis	Paulina	Inorganic and Organic Chemistry	Inorganic Chemistry
Piqué Caufapé	Oriol	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

Echeverría López	Jorge	Inorganic and Organic Chemistry	Inorganic Chemistry
Morales García	Ángel	Materials Science & Physical Chemistry	Physical Chemistry
Wang	Binju	Inorganic and Organic Chemistry	Organic Chemistry

Marie-Curie

Albareda Piquer	Guillem	IQTCUB	

Ramón y Cajal

Calle Vallejo	Federico	Materials Science & Physical Chemistry	Physical Chemistry
Viñes Solana	Francesc	Materials Science & Physical Chemistry	Physical Chemistry

Contracte Projecte de Recerca

Bahamón	Daniel	Materials Science & Physical Chemistry	Physical Chemistry
Güell Riera	Oriol	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

Hjorth Larsen	Ask	Materials Science & Physical Chemistry	Physical Chemistry
Lamiel Garcia	J. Oriol	Materials Science & Physical Chemistry	Physical Chemistry
Vilà Casanova	Arnau	Materials Science & Physical Chemistry	Physical Chemistry

Ph.D. Students

FI Grant (Catalan Government Program)

Balcells Nadal	Cristina	Materials Science & Physical Chemistry	Physical Chemistry
Blanco Andrés	Pablo Miguel	Materials Science & Physical Chemistry	Physical Chemistry
Nin Hill	Alba	Inorganic and Organic Chemistry	Organic Chemistry
Prats García	Hèctor	Materials Science & Physical Chemistry	Physical Chemistry

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

Bernuz Fitó	Efrem	Materials Science & Physical Chemistry	Physical Chemistry
Climent Biescas	Clàudia	Materials Science & Physical Chemistry	Physical Chemistry
Coines López-Nieto	Joan	Inorganic and Organic Chemistry	Organic Chemistry
Martín Rodríguez	Alejandro	Inorganic and Organic Chemistry	Inorganic Chemistry
Piñero Vargas	Juan José	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
Mondelo Martell	Manel	Materials Science & Physical Chemistry	Physical Chemistry
Vilaplana Saiz	Marta	Materials Science & Physical Chemistry	Physical Chemistry

ITN UE Grant

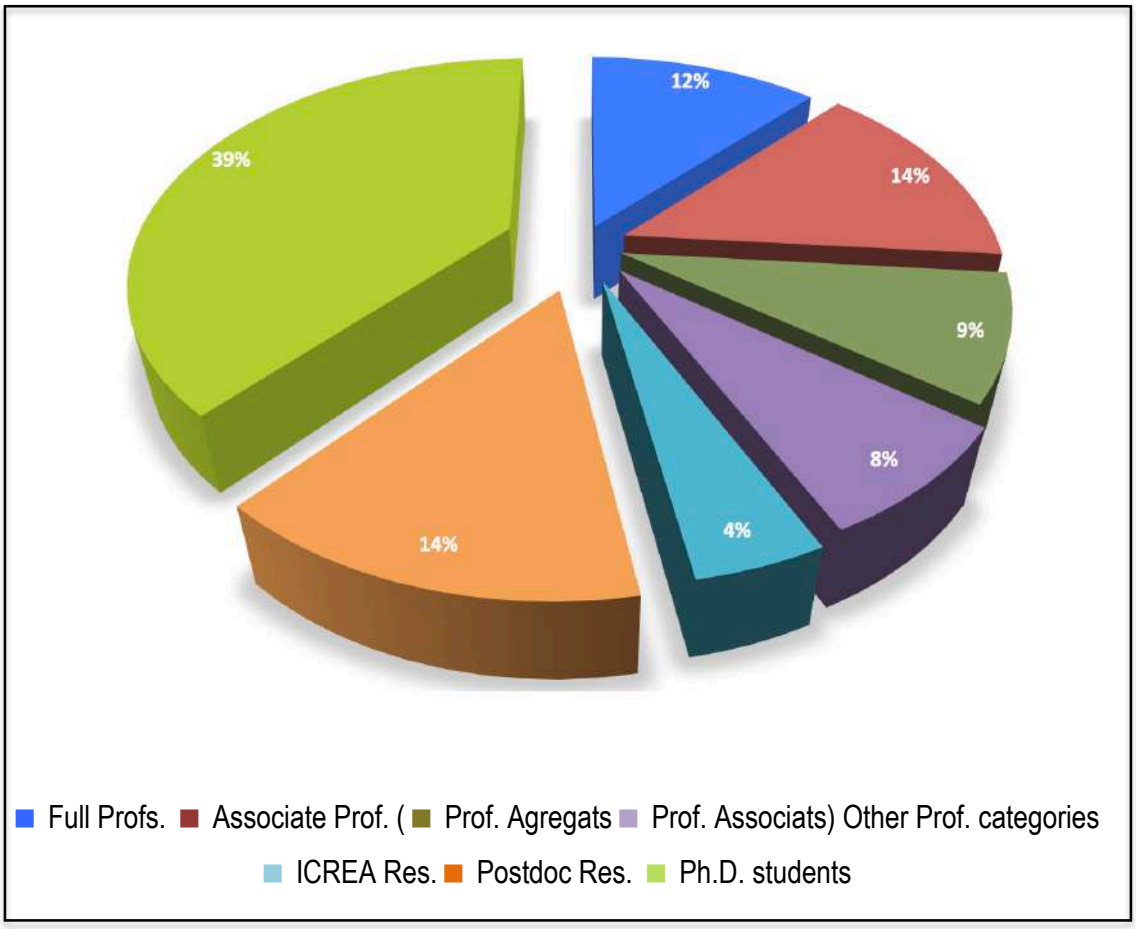
Cuko	Andi	Materials Science & Physical Chemistry	Physical Chemistry
Francese	Tommaso	Materials Science & Physical Chemistry	Physical Chemistry

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
Macià Escatllar	Antoni	Materials Science & Physical Chemistry	Physical Chemistry
Roncero Barrero	Cristina	Materials Science & Physical Chemistry	Physical Chemistry

Other

De Moya	Natalia	Materials Science & Physical Chemistry	Physical Chemistry
Figueroba Sánchez	Alberto	Materials Science & Physical Chemistry	Physical Chemistry
Gómez Mudarra	Francisco	Inorganic and Organic Chemistry	Inorganic Chemistry
Kamalinahad	Saedeh	Materials Science & Physical Chemistry	Physical Chemistry
Keshavarz	Sarah	Materials Science & Physical Chemistry	Physical Chemistry
Lidmar von Ranke	Natalia	Materials Science & Physical Chemistry	Physical Chemistry
López Berbel	Martí	Materials Science & Physical Chemistry	Physical Chemistry
Lozano Reis	Pablo	Materials Science & Physical Chemistry	Physical Chemistry
Muñoz Galán	Helena	Materials Science & Physical Chemistry	Physical Chemistry
Patel Vijaykumar	Mitali	Inorganic and Organic Chemistry	Inorganic Chemistry
Privat Contreras	Cristian	Materials Science & Physical Chemistry	Physical Chemistry
Raich Armendáriz	Lluís	Inorganic and Organic Chemistry	Organic Chemistry
Svobodova	Adela	Materials Science & Physical Chemistry	Physical Chemistry
Vega Domínguez	Lorena	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 nine calculation clusters located in two conditioned rooms of the Chemistry and Physics Faculty of UB. All the clusters except iqtc06 and iqtc07 are located in a room near the garage of the faculty where it is cooled by two air conditioning machines of 47,000 and 66,000 KW, respectively. Iqtc06 and Iqtc07 are located in a room called VAX, which is cooled by one 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: 1,80 GHz Opteron Dual processor (64bits)
RAM: 8 GB
HD: 1 x 146 GB hard disk + 2,5 TB direct attached storage
Network: 2 gigabit network cards (one for external network and one for calculation network)

7 Sun Fire V60X nodes (3,06 GHz processor)
CPU: 3,06 GHz Xeon Dual processor (32 bits)
RAM: 3 GB
HD: 2 x 36 GB hard disk
Network: 2 gigabit network cards (calculation network)

92 Sun Fire V60X nodes (2,80 GHz processor)
CPU: 2,80 GHz Xeon Dual processor (32 bits)
RAM: 6 nodes with 4 GB, 86 nodes with 3 GB
HD: 2 x 36 GB hard disk
Network: 2 gigabit network cards (calculation network)

11 Sun Fire V20Z nodes (1,80 GHz processor)
CPU: 1,80 GHz Opteron Dual processor (64 bits)
RAM: 10 nodes with 8 GB, 2 nodes with 16 GB
HD: 10 nodes with 2 x 73 GB hard disk, 2 nodes with 2 x 73GB and 2 x 300 GB hard disk respectively
Network: 2 gigabit network cards (calculation network)

1 Sun Fire V20Z node 64 bits (2,20 GHz processor)
CPU: 2,20 GHz Opteron Dual processor (64 bits)
RAM: 16 GB
HD: 2 x 146 GB 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: 2 x 2,2 GHz AMD Opteron 275 Dualcore
RAM: 8 GB
HD: 2 x 80 GB 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: 2 x 2,66 GHz Xeon QuadCore
RAM: 16 GB
HD: 2 x 250 GB hard disk
Network: 2 gigabit network card (calculation network) + 1 ILO card (OOB)

5 INTEL HP ProLiant DL160 G5 nodes
CPU: 2 x 2,66 GHz Xeon QuadCore
RAM: 16 GB
HD: 4 x 250 GB hard disk
Network: 2 gigabit network card (calculation network) + 1 ILO card (OOB)

1 INTEL HP ProLiant DL160 G5 node
CPU: 2 x 2,66 GHz Xeon QuadCore
RAM: 16 GB
HD: 2 x 500 GB hard disk
Network: 2 gigabit network card (calculation network) + 1 ILO card (OOB)

3 INTEL HP ProLiant DL160 G5 nodes
CPU: 2 x 2,66 GHz Xeon QuadCore
RAM: 32 GB
HD: 2 x 250 GB 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: 2 x 2,33 GHz Xeon QuadCore
RAM: 16-32 GB
HD: 2 x 80 GB 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: 2 x 2,66 GHz Xeon SixCore
RAM: 48 GB
HD: 1 x 1 TB 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: 2 x 2,66 GHz Xeon SixCore
RAM: 48 GB
HD: 4 x 500 GB 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: 2 x 2,66 GHz Xeon SixCore
RAM: 48 GB
HD: 1 x 500 GB 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: 4 x 2,3 GHz Opteron 6276 16-core
RAM: 256 GB
HD: 2 x 1 TB 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	32 nodes
Notes	64 bits processors

Specifications:

25 INTEL HP ProLiant DL560 Gen8 nodes
CPU: 4 x 2,2 GHz Xeon OctoCore
RAM: 512 GB
HD: 2 x 300 GB hard disk
Network: 4 gigabit network card (calculation network) + 1 IPMI card (OOB)
Network: 2 x 10 gigabit network card (internal data network)

7 INTEL Supermicro SuperServer 8017R-TF+
CPU: 4 x 2,3 GHz Xeon OctoCore
RAM: 512 GB
HD: 3 x 1 TB hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (OOB)
Network: 2 x 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: 4 x 2,6 GHZ Intel Broadwell 10Core
RAM: 512 GB or 1 TB
HD: 1 x 1 TB hard disk
Network: 4 gigabit network card (calculation network) + 1 IPMI card (OOB)
Network: 2 x 10gigabit network card (internal data network)

iqtc08 (*invested value 155.000 €*)

Machine type	HP Cluster
Operating System	Centos 7.2
Services	Calculation cluster
Structure	21 nodes
Notes	64 bits processors

Specifications

21 HP Proliant DL360 Gen9
CPU: 2 x 2,6 GHz Intel Xeon E5-2690 v4 14-core
RAM: 768 GB
HD: 1 x 1 TB hard disk
Network: 4 gigabit network card (calculation network) + 1 IPMI card (OOB)
Network: 2 x 10gigabit network card (internal data network)

GPU cluster (*invested value 57.000 €*)

Machine type	Heterogeneous Cluster
Operating System	SLES11, centos 7

Services	Calculation cluster with GPUs
Structure	*5* nodes
Notes	64 bits processors

Specifications:

Node
CPU: 1 x 3,06 GHz Intel Core i7 950
RAM: 16 GB
HD: 1 x 1 TB hard disk
Network: 1 gigabit network card (calculation network)
GPU: 1 NVIDIA GTX580, 1 NVIDIA GTX480

Node Tyan FT72B7015
CPU: 2 x 2,66 GHz Xeon SixCore
RAM: 48 GB
HD: 1 x 500 GB hard disk
Network: 4 gigabit network card (calculation network) + 1 IPMI card (OOB)
GPU: 8 NVIDIA GTX580

Node
CPU: 1 x 3,30 GHz AMD FX-4100 QuadCore
RAM: 16 GB
HD: 1 x 1 TB hard disk
Network: 1 gigabit network card (calculation network)
GPU: 1 NVIDIA GTX770

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

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

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

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

Node SIE LADON BROADWELL 2
CPU: 2 x 2,4 GHz Xeon E5-2640v4
RAM: 128 GB
HD: 1 x 1 TB hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (OOB)
GPU: 2 NVIDIA TESLA P100

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: 2 x 2,50 GHz Xeon QuadCore E5420
RAM: 8 GB
HD: 4 x 1 TB (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: 2 x 2,27 GHz Xeon QuadCore E5520
RAM: 56 GB
HD: 12 x 2 TB (raid 5)
Network: 2 gigabit network card (internal network) + 1 IPMI card (OOB)

1 INTEL HP ProLiant DL380e Gen8 node
CPU: 2 x 2,20 GHz Xeon QuadCore E5-2407
RAM: 48 GB
HD: 12 x 2 TB (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: 1 x 2,33 GHz Xeon Dual Core
RAM: 8 GB
HD: 1 x 160 GB 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: 2 x 2,50 GHz Xeon QuadCore E5420
RAM: 8 GB
HD: 2 x 1 TB (raid 1)
Network: 3 gigabit network card (internal network)

2 INTEL HP ProLiant DL120 G5 node
CPU: 1 x 2,33 GHz Xeon Dual Core
RAM: 8 GB
HD: 2 x 160 GB 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 : 2 x 2,2 GHz AMD Opteron 275 Dualcore
RAM: 4 GB
HD: 6 x 146 GB 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).
11. 2 Switch Netgear XS728T 10GB (internal and calculation network for iqtc08).
12. 1 Switch HPE 1810-24 (internal network iqtc08).

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

SUMMARY

Cores.....3,994 c

Memory ..... 27,816 GB RAM

Calculation disk capacity..... 199 TB

Data user disk capacity.....32 TB

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

*2.028.000 €**

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

IQTCUB's iqtc08 CPU cluster (left) and GPU cluster (right)

II. IQTCUB ACTIVITIES

II.1 GENERAL ACTIVITIES

Next, a description of activities and actions promoted by IQTCUB through 2017 is provided.

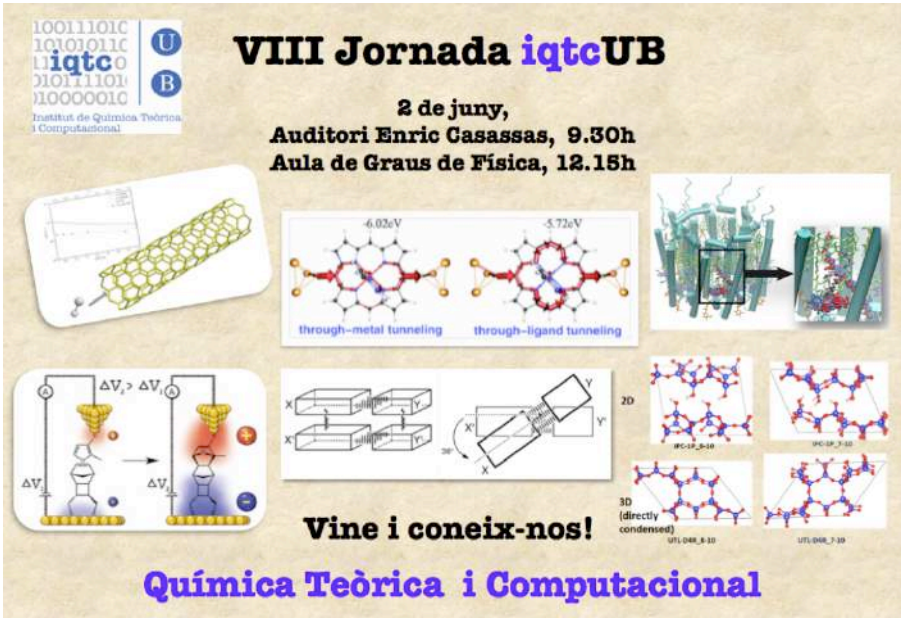
a. ***Promotion and encouragement of research.*** This year the IQTCUB has finally offered three contracts (around 2000 € per contract) aimed to help students to initiate a scientific career. These contracts are addressed to students about to end the degree and aimed to cover a six-month period to facilitate 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 Biel Martínez Díaz, Pablo Lozano Reis and Cristian Privat Contreras for starting Master studies under the supervision of Drs. Fermín Huarte, Pablo Gamallo and Jaime Rubio, respectively.

Total cost: 6.246 €

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

b. ***8th IQTCUB workshop.*** This one-day workshop aimed at the dissemination of the research done at the IQTCUB took place on July 2nd, 2017 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. Dr. Carmen Herrmann from the Universität Hamburg with the invited lecture entitled *Pathways in molecular conductance and spin coupling*, Dr. Carles Curutchet (*Multiscale modelin of light harvesting and energy transfer in photosynthesis*), Manel Mondelo (*The importance of the tunnel effect on the diffusion of H_2 along a SWCNT*), Dr. Jordi Poater (*Chemically-controlled DNA nanoswitch*), Ángel Morales-García (*Effect of the pressure on the synthesis of ADOR zeolites*) and Dr. Ismael Díez (*Tailoring the electrical behavior of a single molecule contact*) from the University of Barcelona and IQTCUB. Moreover, 15 poster contributions have been presented during the meeting. The IQTCUB assigned a budget to cover the traveling and lodging expenses of Prof. Dr. Carmen Herrmann as well as the catering service offered to all assistants.

Total cost: 1.730 €



Panel of the *8th IQTCUB workshop*.

c. ***7th 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 2017 edition has been the seventh 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 Antoni Macià (UB, IQTCUB).
2. *Visualising Biomolecules,* Drs. Carme Rovira, Alba Nin, Joan Coines and Binju Wang (UB, IQTCUB).
3. *Structured Programming,* Profs. Albert Solé and J. Carlos Paniagua (UB, IQTCUB).
4. *Cellular Automaton,* Prof. Pere Alemany and Efrem Bernuz (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).

The present edition took place from June 26th to 30th, and 15 students performed the course.

Total cost: 250 €

Panel of the 7th *Introductory Course in Computational Chemistry* held in 2017.

d. ***6th 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 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 3rd to 7th. 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: C. Vilar, N. Górriz, P. Lozano, E. Braña, R. Santiago, M. Condeminas, A. González, M. Peralta, R. Morales, P. Llinares, L. Castilla, R. Herrera, M. Torres, O. Gómez and M. Cortes. 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. *Excited states,* Prof. Mercè Deumal (UB, IQTCUB).

5. *Introduction to SGE,* Jordi Inglés and Teresa Arenal *(IQTCUB computing technicians).*

6. *Solid state,* Profs. Iberio Ribeiro (UB, IQTCUB).

7. *Fortran 90,* Prof. Miquel Llunell (UB, IQTCUB).

Panel of the 6th *Advanced Course in Computational Chemistry* held in 2017.

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 2017 the periodic *IQTC Internal Seminars* have continued. Those seminars are given 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, both 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 2017:

1. *Influence of the sulfur bridge in the photophysics of covalent naphthalene dimers.*

   Claudia Climent, January 20, 2017.
2. *BASH: Not only terminal commands, but also a programming language.*

   Gerard Alonso, January 20, 2017.
3. *How to give successful talks*.

   Prof. Stefan T. Bromley, March 3, 2017.
4. *Effect of Si/Al ratio on CO_2 capture by adsorption with faujasites and application in engineering processes.*

   Ph.D. Daniel Bahamon, April 28, 2017.
5. *Modelling the reaction intermediate of glycoside hydrolases.*

   Joan Coines, April 28, 2017.
6. *Introducció a l'aproximació GTD (no és de Química Quàntica, és d'organització personal).*

   Prof. Albert Solé, June 9, 2017.
7. *Enzymes with biotechnological applications.*

   Lluís Raich, July 21, 2017.
8. *Experimental and theoretical points of view of Li+ i-C_3H_7Br gas-phase reaction.*

   Ph.D. Estefanía López, July 21, 2017.
9. *Dynamics of reactions inside superfluid Helium nanodroplets.*

   Miquel Blancafort, October 6, 2017.
10. *Astronomical Dust: Origin, importance and current knowledge.*

    Antoni Macià, October 6, 2017.
11. *Unraveling brain diseases using QM/MM methods: Catalytic study of b-galactocerebrosidase.*

    Alba Nin, November 17, 2017.
12. *Discovery of novel silicon carbonate (SiCO) at high pressure.*

    Ph.D. Angel Morales, November 17, 2017.

f. ***Scientific Dissemination Activities.*** Prof. Xavier Giménez Font has been involved in the following scientific and teaching dissemination activities during 2017:

1. "*UB s'Apropa 17*".
   Europa International School Sant Cugat del Vallès, January 16, 2017.
   Institut Manuel Blancafort, La Garriga, January 17, 2017.
   Escola Pia de Granollers, Granollers, January 27, 2017.
   Escola Pia de Caldes, Caldes de Montbui, January 30, 2017.
   Escola Municipal del Treball, Granollers, February 1, 2017.
   Institut La Vall del Tenes, Sta. Eulàlia de Ronsana, February 3, 2017.
   Institut Maria de Bell–Lloc, Bigues i Riells, February 6, 2017.
   Institut Alba del Vallès, Sant Fost de Campsentelles, February 8, 2017.
   Alba del Vallès, Sant Fost de Campsentelles, February 9, 2017.
2. "*Active Learning Education in Science*", Round Table in "**Jornada d'Investigadors Predoctorals Interdisciplinària**". Universitat de Barcelona, Barcelona, February 9, 2017.
3. "*UB s'Apropa 17*".
   Institut La Roca del Vallès, La Roca del Vallès, February 10, 2017.
   Institut Vilanova del Vallès, Vilanova del Vallès, February 10, 2017.
   Institut Vilanova del Vallès, Vilanova del Vallès, February 10, 2017.
   Institut Moianès, Moià, February 16, 2017.
   Institut Mollet del Vallès, Mollet del Vallès, February 17, 2017.
   Institut El Sui, Cardedeu, February 21, 2017.
   Jesuïtes Sant Gervasi – Escola Infant Jesús, Barcelona, February 22, 2017.
   Institut El Sui, Cardedeu, February 23, 2017.
   Institut Milà i Fontanals, Vilafranca del Penedès, March 1, 2017.
   Institut Camí de Mar, Calafell, March 2, 2017.
4. "*L'Aire que respirem*". **Toc–Toc UB Science Dissemination Program**, Institut Manuel Blancafort, La Garriga, March 30, 2017.
5. "*UB s'Apropa 17*".
   Institut Manolo Hugué, Caldes de Montbui, April 7, 2017.
6. "*L'Aire que Respirem*". **Toc–Toc UB Science Dissemination Program,** Escola Municipal del Treball, Granollers, April 19, 2017.

7. "*Hagamos posible el buen rendimiento académico*", 4–hour course at Universidad de Extremadura, Cáceres, May 4, 2017.
8. "*Les Microones i les Ones de Ràdio: què són i com ens afecten?*". **Toc–Toc UB Science Dissemination Program,** Centre Cultural Sant Josep — Jornades "Pessics de Ciència", Hospitalet de Llobregat, May 17, 2017.
9. "*The role of Universities in the Energy Transition: multidisciplinary education and research*". **5th Uni–SET Meeting**. KU Leuven, Leuven, Belgium, June 2, 2017.
10. "*Ensenyar a aprendre: millorem l'aprenentatge de les ciències i la tecnologia*", 8–hour course at Universitat de Lleida, Lleida, June 5, 2017.
11. "*Profesores de Ciencias, hagamos posible el buen rendimiento académico sin clases magistrales*", 8–hour course at Universidad de Sevilla, Sevilla, June 19–20, 2017.
12. "*El mètode SABER de classe invertida síncrona en un entorn STEM*". One–day meeting "**L'enfocament d'aula inversa a la Universitat**", Universitat de Girona, June 21, 2017.
13. "*Let's make high academic performance possible*". Workshop ***Learnin's Creatin'***. Instituto Politécnico de Viseu, Viseu, Portugal, September 13–14, 2017.
14. "*Practical strategies to improve students' performance, with emphasis on STEM: the SABER synchronous flipped classroom*". Conference at **"*1st international conference in experiences in active learning in higher education*"**, Facutat d'Economia i Empresa, Universitat de Barcelona, October 27, 2017.
15. "*Llibres de Divulgació Científica*", Màster de Comunicació Científica, Univ. Barcelona, November 13, 2017.
16. "*L'Aire que Respirem*", **La Setmana de la Ciència**, Institut Joan Brudieu, La Seu d'Urgell, November 15, 2017.
17. "*La màgia de l'aigua*", **La Setmana de la Ciència**, Sala Noble de Can Rius, Caldes de Montbui, November 17, 2017.
18. "*UB s'Apropa 18*".
    La Salle Manresa, Social Science Students, Manresa, Novembre 24, 2017.
    La Salle Manresa, Science Students, Manresa, November 24, 2017.

19. "*L'Aire que Respirem*". **Toc–Toc UB Science Dissemination Program,** Oak House School, Barcelona, November 29, 2017.
20. "*L'Aire que Respirem*". **Toc–Toc UB Science Dissemination Program,** Biblioteca Sagrada Família, Barcelona, November 29, 2017.
21. "*Enseñar a aprender: de las clases magistrales a la clase invertida síncrona*", Openning Lecture at **IV Jornadas de Docencia Universitaria** de la Universidad de Sevilla, Sevilla, December 4–5, 2017.

Moreover, Prof. Giménez has been interviewed in different media:

1. "*Education in Science*" Discussion at JIPI'17, Jornada d'Investigadors Predoctorals Interdisciplinària. **UBTV**, Universitat de Barcelona, February 9, 2017 (http://www.ub.edu/ubtv/video/debate-education-in-science).
2. "*Can Barcelona superblocks cut traffic and clean up city air?*" Interview by Sophie Davies, United States edition of **Reuters.com**, February 23, 2017 (http://www.reuters.com/article/us-spain-urban-pollution-transport-idUSKBN1621E7).
3. "*Què és la felicitat*" Interview by Guillem Martínez, Science section of **BTV**, March 20, 2017 (http://beteve.cat/seccions/tecnologia/).
4. "*Dormir a prop del mòbil: entre el risc i la falsa alarma*". Interview by Marc Garcia, Life section of **El Món**, March 25, 2017 (http://elmon.cat/noticia/192028/dormir-a-prop-del-mobil-entre-el-risc-i-la-falsa-alarma).
5. "*La polémica solución de Trump al cambio climàtico: lanzar productos químicos al aire*". Interview by Rocío Pérez Benavente, Science section of **El Confidencial**, March 29, 2017 (http://www.elconfidencial.com/tecnologia/ciencia/2017-03-29/geoingenieria-solar-cambio-climatico-quimicos-atmosfera_1356072/).
6. "*La contaminació de l'aire que respirem al Vallès Oriental*". Interview by Dani Agudo for Infovallès, **VOTV**, April 19, 2017 (http://votv.xiptv.cat/entrevista#).
7. "*Dudas sobre la efectividad de las medidas anticontaminación*". Interview by Pablo Alegre, Mobility section, **Metrópoli Abierta Barcelona**, April 20, 2017 (http://www.metropoliabierta.com/el-pulso-de-la-ciudad/movilidad/restringir-acceso-barcelona-problemas-soluciones-contaminacion_1055_102.html).

8. "*Ha pujat l'ús de mascaretes antipol·lució. Són efectives?*". Interview by Miriam Santamaria, program **Verd Primera**, **BTV**, May 10, 2017 (http://beteve.cat/clip/entrevista-a-xavier-gimenez-i-pau-girbau-sobre-les-mascaretes-antipollucio/).
9. "*Les microones i les ones de ràdio: què són i com ens afecten*". Conference within the series "**Pessics de Ciència**", Centre Cultural Sant Josep, L'Hospitalet de Llobregat, May 17, 2017 (https://www.youtube.com/watch?v=UKEhCROFrhk).
10. "*El termòmetre i el mercuri*", Interview by Marta Ballesta, Program "Les 10 notícies", **BTV**, June 16, 2017 (http://beteve.cat/programa/les-10-noticies/).
11. *"La contaminació atmosfèrica"*. Interview by Martí Roma et al, for a **newsgame within a Degree Final Report** (TFG), Journalism Degree, Universitat Pompeu Fabra, Barcelona (http://verdalia.cat/).
12. "*El mètode SABER de classe invertida síncrona en un entorn STEM*". One–day meeting "**L'enfocament d'aula inversa a la Universitat**", Universitat de Girona, June 21, 2017 (http://diobma.udg.edu/handle/10256.1/4836).
13. "*L'Aire que Respirem*". Talk at INS Joan Brudieu, La Seu d'Urgell, during "La Setmana de la Ciència 2017", November 15, 2017 (https://www.youtube.com/watch?v=nxWkozNzWYk).

II.2 IQTCUB SEMINARS AND CONFERENCES

Dr. Stefan Bromley has continued organizing the seminars and conferences of IQTCUB during 2017. A total of ten seminars and/or conferences, which are listed below:

1. **Prof. Manuel Alcamí** (Universidad Autónoma de Madrid), Madrid, Spain.
   Nanoestructuras de carbono modificadas por la interacción con metales: ¿Qué nos aportan los cálculos teóricos?
   January 12, 2017.

2. **Prof. Sebastien Thibaudeau** (Institut de Chimie des Milieux et Matériaux de Poitiers, Université de Poitiers) Poitiers, France.
   Superelectrophilic activation in superacid media: how to predict it?
   February 14, 2017.

3. **Dr. Monica Calatayud** (Laboratoire de Chimie Théorétique, Université P. M. Curie), Paris, France.
   Ab initio modelling of materials: role of surfaces in reactivity.
   March 30, 2017.

4. **Dr. Adriana Isvoran** (Dept. Biology-Chemistry and Advanced Environmental Research Laboratories, West University of Timisoara), Timisoara, Romania.
   Chemoinformatics of xenobiotics.
   April 20, 2017.

5. **Prof. J. Peter Toennies** (Max Plank Institute for Dynamics and Self-Organization), Göttingen, Germany.
   Enigmatic molecules of helium and molecules in enigmatic helium.
   April 26, 2017.

6. **Dr. Rubén Pérez** (Universidad Autónoma de Madrid), Madrid, Spain.
   Adatoms, polarons and the catalytic activity of ceria: microscopic insights from first principles calculations.
   May 25, 2017.

7. **Michael Nolan** (Tyndall National Institute), Cork, Ireland.
   Functional metal oxide surfaces and interfaces.
   October 5, 2017.

8. **Prof. Jong Min Lee** (Nanyang Technological University) Singapore.
   Ionic liquids and their applications.
   October 19, 2017.

9. **Prof. Mariona Sodupe** (Universitat Autònoma de Barcelona), Barcelona, Spain.
   Mineral induced prebiotic chemical processes. Insights from computational approaches.
   November 16, 2017.

10. **Dr. Daniel Reta** (University of Manchester), Manchester, United Kingdom.
    Molecular magnetic hysteresis at 60 K in dysprosocenium.
    October 23, 2017.

II.3 IQTCUB INVITED RESEARCHERS

During 2017, a total of seven researchers from all over the world have spent some time at the IQTCUB collaborating in different research projects.

1. **Fatemeh Keshavarz** (invited visitor).
   College of Science, Shiraz University, Shiraz, Iran.
   September 2016 - May 2017.

2. **Haruna Luz Barazorda Ccahuana** (invited visitor).
   Universitat Catòlica de Santa Maria de Arequipa, Yanahuara, Peru.
   August - November 2017.

3. **Prof. Hristiyan Alesandrov** (invited visitor).
   University of Sofia, Sofia, Bulgaria.
   January - February, July-August 2017.

4. **Prof. Jorge Pavez** (invited visitor).
   Universitat de Santiago de Chile, Chile.
   December 2017.

5. **Lorenzo Zamirri** (invited visitor).
   Universitat de Torino, Torino, Italy.
   December 2017.

6. **Dr. Miroslava Nedyalkova** (Materials networking European project).
   University of Sofia, Sofia, Bulgaria.
   February - March, July - August 2017.

7. **Saedeh Kamalinahad** (invited visitor).
   Department of Chemistry, Arak University, Arak, Iran.
   August 2017 - February 2018.

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

An algorithm to Locate Optimal Bond Breaking Points on a Potential Energy Surface for Applications in Mechanochemistry and Catalysis

J. M. Bofill, J. Ribas-Ariño, S. P. García, W. Quapp.

J. Chem. Phys., *147* (2017) 152710.

$$\text{Optimal Bond Breaking Point conditions} \begin{cases} \mathbf{H}(\mathbf{x}_{optBBP})\mathbf{g}(\mathbf{x}_{optBBP}) = \mathbf{0} \\ \mathbf{g}(\mathbf{x}_{optBBP}) \neq \mathbf{0} \end{cases}$$

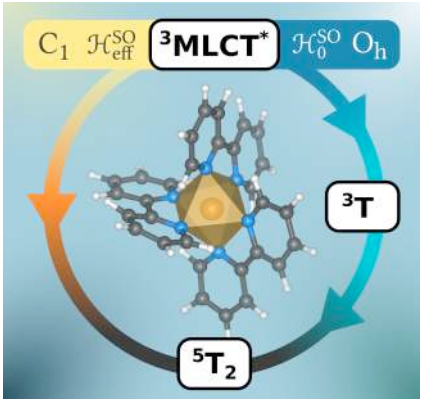
Given a reactive molecular system, a well-fitted pulling direction, and a sufficiently large value of the force, the minimum configuration of the reactant and the saddle point configuration of a transition state collapse at a point on the corresponding reaction path. This point is called bond breaking point (BBP). The Hessian matrix at the BBP has a zero eigenvector, which coincides with the gradient. It indicates which force (both in magnitude and direction) should be applied to the system to induce the reaction in a barrierless process. Within the manifold of BBPs, there exist *optimal BBPs*, which indicate what is the optimal pulling direction, and what is the minimal magnitude of the force to be applied for a given mechanochemical transformation. Since these special points are very important in the context of mechanochemistry and catalysis, a Gauss-Newton algorithm was proposed for their location.

LINE 2. COMPUTATIONAL MATERIALS SCIENCE

Effect of Second-Order Spin-Orbit Coupling on the Interaction between Spin States in Spin-Crossover Systems

C. Sousa, A. Domingo, C. de Graaf.

Chem. Eur. J., *23* (2017) 1.



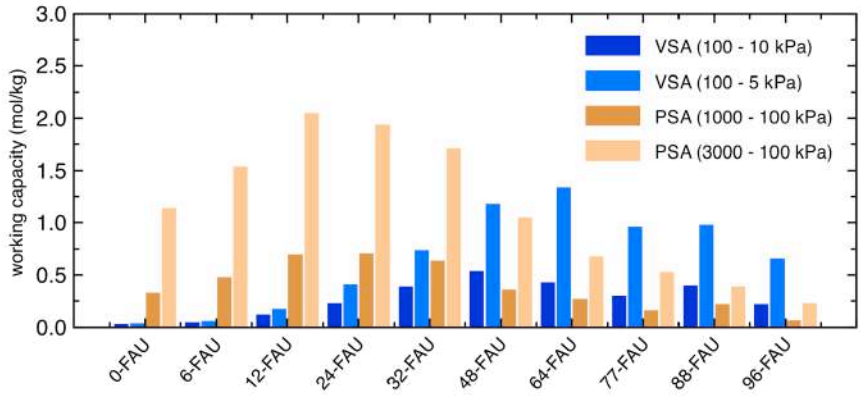
Inclusion of second-order spin-orbit coupling and geometrical distorsions explains the mechanism of the light-induced spin crossover.

The second-order spin-orbit coupling is evaluated in two transition-metal complexes to establish the effect on the deactivation mechanism of the excited low-spin state in systems that undergo spin transitions under the influence of light. The combined effect of geometry distortions and second-order spin-orbit coupling leads to sizeable interactions for states that are nearly uncoupled in the symmetric (average) structure of the complex. This opens the possibility of a direct deactivation from the singlet and triplet states to the metal-to-ligand charge-transfer manifold and to the final high-spin state as suggested from the interpretation of experimental data but so far not supported by theoretical descriptions of the light-induced spin crossover.

Optimal Faujasite structures for post combustion CO_2 capture and separation in different swing adsorption processes

H. Prats, D. Bahamón, G. Alonso, X. Giménez, P. Gamallo, R. Sayós.

J. CO_2 Util., *19* (2017) 100.



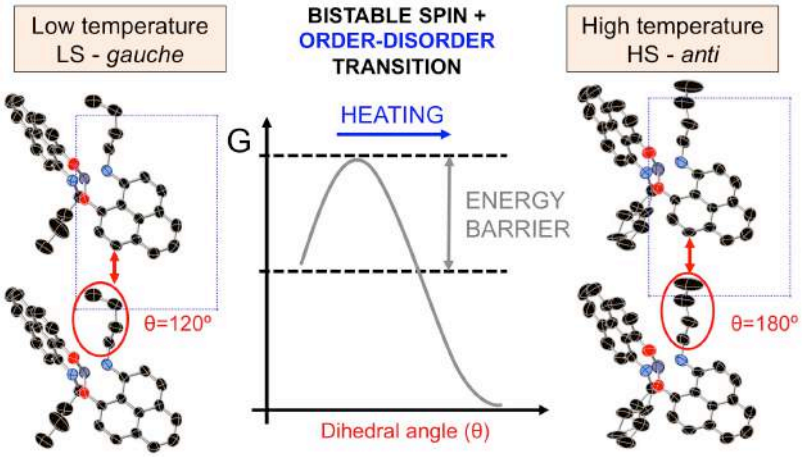
Calculated CO_2 working capacities for the ten FAU structures considered corresponding to PSA and VSA processes at different pressures and at 313 K.

Grand Canonical Monte–Carlo simulations are used in this work, to assess optimum faujasite structures in CO_2 capture processes. Pressure Swing Adsorption (PSA) and Vacuum Swing Adsorption (VSA) procedures have been considered to evaluate purity, working capacity and breakthrough time. To this purpose, ten faujasite structures with different Al content were selected, and the best conditions for CO_2 capture maximization have been calculated for each structure. Further results show that zeolites having intermediate Al content are the most effective for VSA processes, whereas low Al content faujasites perform better at PSA conditions. Remarkably, present work best results clearly improve faujasite 13X VSA–PSA performances, so far considered the industrial reference in absence of water. Moreover, combined VPSA processes, in terms of working capacity and adiabatic work required for compression/expansion, have also been studied, showing that VPSA systems are more efficient than pure PSA/VSA, for structures with intermediate Al content. Finally, an improved methodology has been derived, where mixture isotherms and energetic cost calculations are combined, and a more accurate way of estimating working capacities and breakthrough times is proposed.

Origin of bistability in the butyl-substituted spirobiphenalenyl-based neutral radical material

M. Fumanal, J. J. Novoa, J. Ribas-Ariño.

Chem. Eur. J., *23* (2017) 7772.

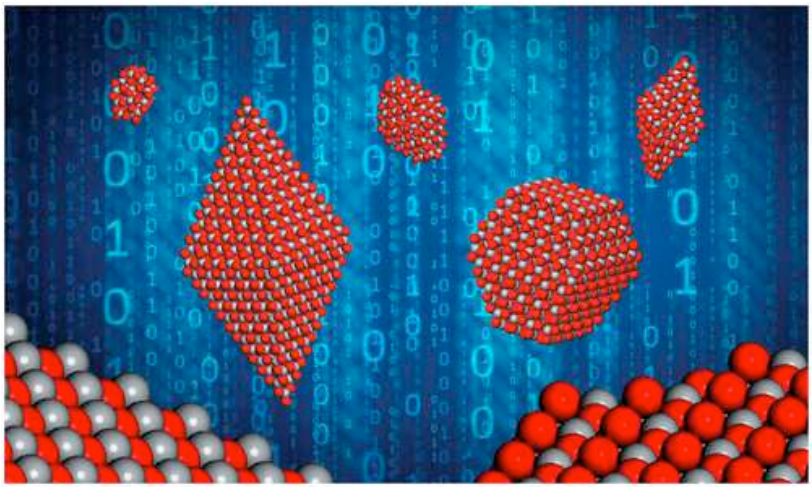


One of the most remarkable bistable materials reported so far is made of π dimers of a butyl-substituted spirobiphenalenyl boron radical (butyl-SBP). The phase transition of this material, which is accompanied by changes in its optical, conductive, and magnetic properties, occurs with a hysteretic loop 25 K wide centered at 335 K. In this computational study, we deciphered the origin of this hysteresis. The phase transition of butyl-SBP consists of a spin transition of the constituent π dimers coupled with an order–disorder transition involving the butyl chains linked to phenalenyl rings. Below 335 K, the butyl chains adopt a *gauche* conformation, whereas above 335 K, the butyl chains are in an *anti* conformation and exhibit dynamic disorder. The *gauche* → *anti* conformational rearrangement triggers the spin transition of the π dimers and is responsible for the hysteretic behavior of butyl-SBP. Our results show that coupling a spin switch with a conformational switch provides a promising strategy in the design of new bistable materials.

When Anatase Nanoparticles Become Bulklike: Properties of Realistic TiO_2 Nanoparticles in the 1–6 nm Size Range from All Electron Relativistic Density Functional Theory Based Calculations

O. Lamiel-Garcia, K. C. Ko, J. Y. Lee , S. T. Bromley, F. Illas.

J. Chem. Theory Comput., *13* (2017) 1785.



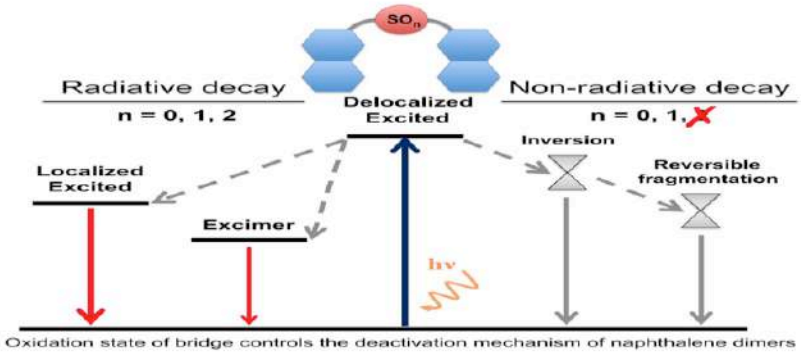
Realistic models of TiO_2 nanoparticles used to study the convergence of properties as a function of size and towards the bulk limit.

All electron relativistic density functional theory calculations on stoichiometric TiO_2 anatase nanoparticles spanning 1–6 nm diameter size, cut following Wulff constructions (Figure), show that their electronic structure properties feature a clear trend converging to bulk values as the nanoparticles size increases, highly influenced by the employed density functional. The electronic structure properties and reactivity for the largest nanoparticles are similar to those exhibited by mesoscale particles or bulk systems. Compelling evidence is presented that anatase nanoparticles become effectively bulklike when reaching a size of ∼20 nm diameter.

The photophysics of naphthalene dimers controlled by sulfur bridge oxidation

C. Climent, M. Barbatti, M. O. Wolf, C. J. Bardeen, D. Casanova.

Chem. Sci. *8* (2017) 4941-4950.



Schematic Jablonski diagram of covalent naphthalene dimers according to the oxidation state of the bridging sulfur (S, SO, SO_2).

In this work we investigate the photophysics of naphthalene dimers covalently linked by a sulfur atom. We explore and rationalize how the oxidation state of the sulfur-bridging atom directly influences the photoluminescence of the dimer by enhancing or depriving its radiative and non-radiative relaxation pathways. In particular, we discuss how oxidation controls the amount of electronic transfer between the naphthalene moieties and the participation of the SO_n bridge in the low-lying electronic transitions. We identify the sulfur electron lone-pairs as crucial actors in the non-radiative decay of the excited sulfide and sulfoxide dimers, which are predicted to proceed *via* a conical intersection (CI). Concretely, two types of CI have been identified for these dimers, which are associated with the photo-induced pyramidal inversion and reverse fragmentation mechanisms found in aryl sulfoxide dimers. The obtained results and conclusions are general enough to be extrapolated to other sulfur-bridged conjugated dimers, therefore proportionating novel strategies in the design of strongly photoluminescent organic molecules with controlled charge transfer.

Oxide-based nanomaterials for fuel cell catalysis: The interplay between supported Pt atoms and particles

Y. Lykhach, A. Bruix, S. Fabris, V. Potin, I. Matolínová, V. Matolín, J. Libuda, K. M. Neyman.

Catal. Sci. Technol., *7* (2017) 4315.

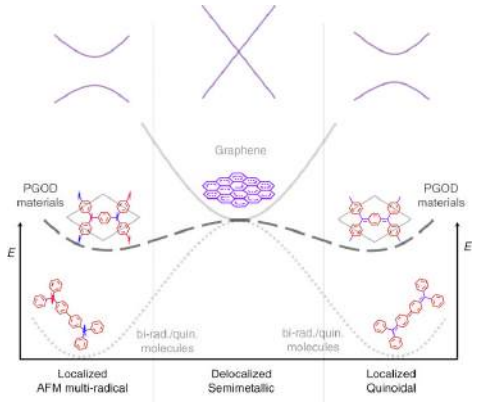
Cover image of the Themed Issue on Single atom catalysis illustrating interplay of single supported on ceria Pt atoms in the catalyst at rest and small Pt clusters formed from such single atoms at the working fuel cell conditions of H_2 dissociation and oxidation.

The concept of single atom catalysis offers maximum noble metal efficiency of low-cost catalytic materials. We presented our experimental and theoretical modelling efforts to fabricate and characterize single atom anode fuel cell catalysts on nanostructured ceria. The remarkable performance and durability of these catalysts with ultra-low Pt loading is related to the interplay between two states associated with supported atomically dispersed Pt and sub-nanometer Pt particles. These two states result from strong interactions between Pt and nanostructured ceria that yield atomic Pt species under oxidizing conditions and small Pt particles under reducing conditions. The square-planar O_4 site on small {100} terraces is the key structural element on the surface of ceria nanoparticles where atomic Pt is anchored as Pt^{2+}. The conversion of Pt^{2+} species to Pt particles is triggered by a redox Ce^{4+}/Ce^{3+} process. The abundance of adsorption sites similar to those on the {100} terraces determines the ideal (maximum) Pt loading in Pt–CeOx films that still allows reversible switching between Pt atoms and small particles yielding high activity and durability of such smart catalysts during fuel cell operation.

Existence of multi-radical and closed-shell semiconducting states in post-graphene organic Dirac materials

I. Alcón, F. Viñes, I. de P. R. Moreira, S. T. Bromley.

Nature Commun., *8* (2017) 1957.

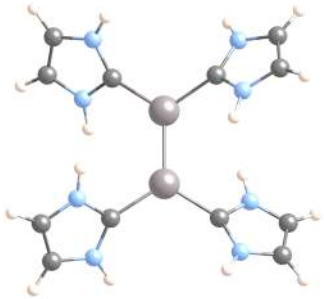


The lack of band gap controllability in graphene severely restricts its use in nanoelectronics. Here, we predict that post-graphene organic Dirac materials should allow for exceptional electronic tunability between graphene-like semimetallicity and multi-radical and/or closed-shell semiconducting states.

Zn-Zn double bonds, a theoretical study

J. Echeverría, A. Falceto, S. Alvarez.

Angew. Chem. Int. Ed., *56* (2017) 10151.



Non-existent Zn-Zn double bonds computationally predicted.

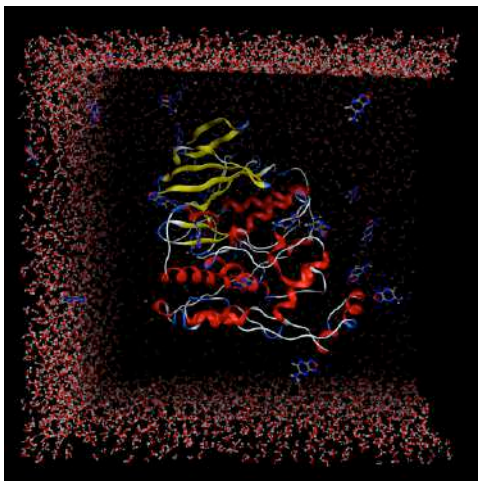
While double bonds are known for transition metals of groups 9 and 10, as well as for boron and p-block elements of groups 14-16, Zn sits in a small region of the periodic table with no well characterized double bonds. A qualitative reasoning indicates that zerovalent Zn has the potential for forming Zn=Zn double bonds. The computational work presented in this paper provides support for such a proposal.

LINE 3. COMPUTATIONAL BIOCHEMISTRY AND *SOFT MATTER*

Identification of Potential Small Molecule Binding Pockets in p38α MAP kinase

P. Gomez-Gutierrez, J. Rubio-Martinez, J. J. Perez.

J. Chem. Inf. Model., *57* (2017) 2566.



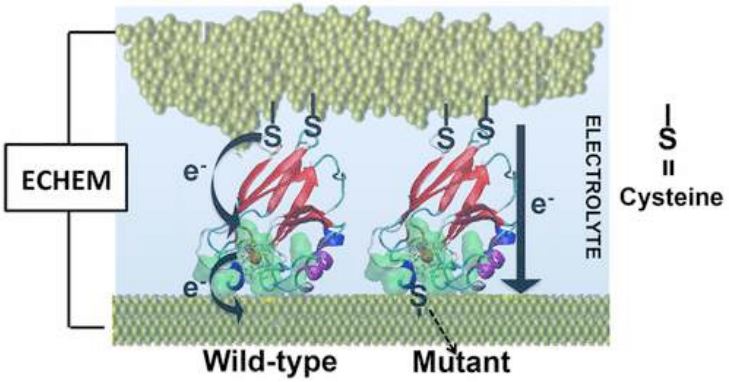
Searching binding pockets using molecular dynamics.

Given the essential role played by protein kinases in regulating cellular pathways, their dysregulation can result in the onset and/or progression of various human diseases. Structural analysis of diverse protein kinases suggests that these proteins exhibit a remarkable plasticity. The present work reports the results of a in silico screening study aimed at identifying novel prospective allosteric binding sites in the paradigmatic p38α MAP kinase. The process was carried out using a protein ensemble generated from a 6 μs accelerated molecular dynamics. The procedure permitted to identify diverse allosteric sites of p38α already described in the literature including the DFG pocket, the lipid binding pocket, the DEF site, the docking groove, the CD and ED sites, the backside site as well as a novel site recently reported: the A-loop regulatory site. Furthermore, the study also permitted to identify ten novel prospective allosteric sites.

Bioengineering a Single-Protein Junction

M. P. Ruiz, A. C. Aragonès, N. Camarero, J. G. Vilhena, M. Ortega, L. A. Zotti, R. Pérez, J. C. Cuevas, P. Gorostiza, I. Díez-Pérez.

J. Am. Chem. Soc.,*139* (2017) 15337.

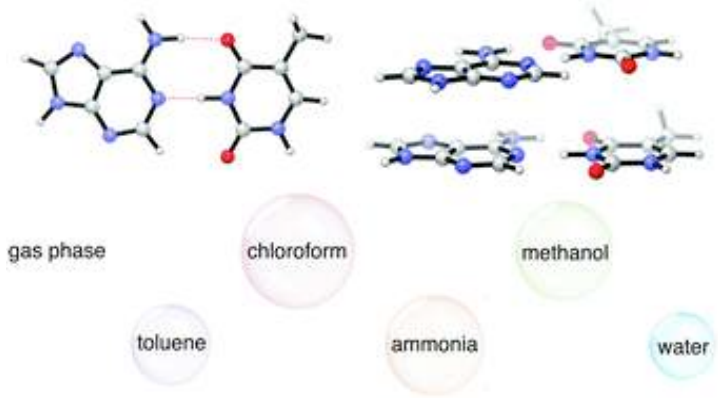


We show here the first example of bioengineered charge transport in a single-protein electrical contact. The results reveal that a single point-site mutation at the docking hydrophobic patch of a Cu-azurin causes minor structural distortion of the protein blue Cu site and a dramatic change in the charge transport regime of the single-protein contact, which goes from the classical Cu-mediated two-step transport in this system to a direct coherent tunneling. This work is a direct evidence of charge transport control in a protein backbone through external mutagenesis and a unique nanoscale platform to study structurally related biological electron transfer.

B-DNA model systems in non-terran bio-solvents: implications for structure, stability and replication

T. A. Hamlin, J. Poater, C. Fonseca Guerra, F. M. Bickelhaupt.

Phys. Chem. Chem. Phys., *19* (2017) 16969.

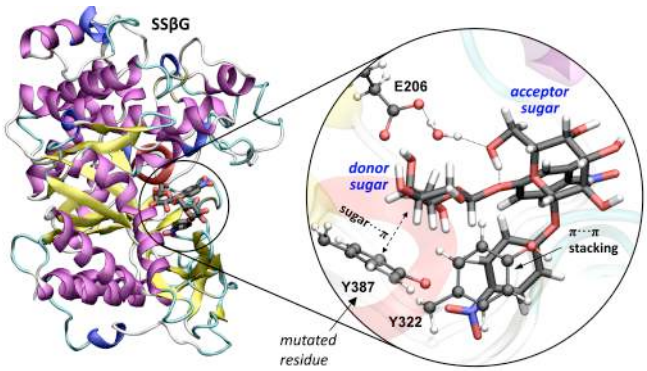


We have computationally analyzed a comprehensive series of Watson–Crick and mismatched B-DNA base pairs, in the gas phase and in several solvents, including toluene, chloroform, ammonia, methanol and water, using dispersion-corrected density functional theory and implicit solvation. Our analyses shed light on how the molecular-recognition machinery behind life's genetic code depends on the medium, in order to contribute to our understanding of the possibility or impossibility for life to exist on exoplanetary bodies. Calculations show how a common non-terran environment like ammonia, less polar than water, exhibits stronger hydrogen-bonding affinities, although showing reduced selectivities towards the correct incorporation of Watson–Crick base pairs into the backbone. Thus, we prove the viability of DNA replication in a non-terran environment.

A Front-Face 'S_Ni synthase' engineered from a retaining 'double-S_N2' hydrolase

J. Iglesias-Fernández, S. M. Hancock, S. S. Lee, M. Khan, J. Kirkpatrick, N. J. Oldham, K. McAuley, A. Fordham-Skelton, C. Rovira, B. G. Davis.

Nat. Chem. Biol., *13* (2017) 874.



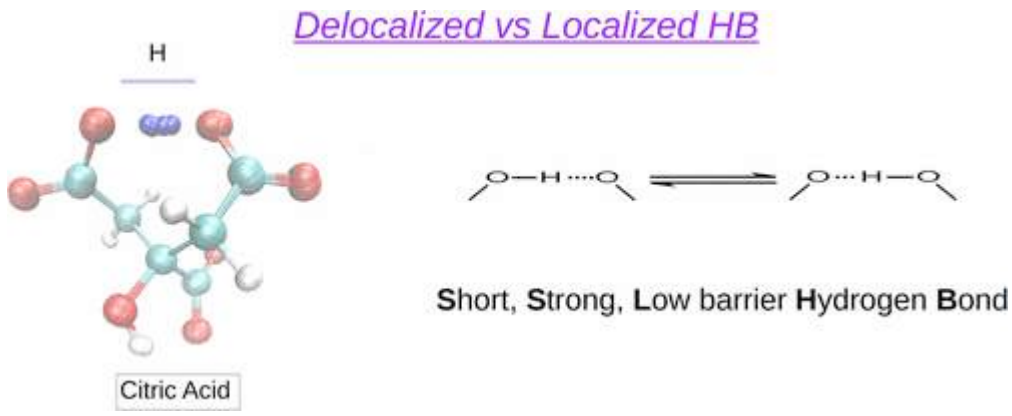
Close view of the active site of the modified enzyme (Sulfolobus solfataricus β-glycosidase, SSβG) showing the two bound carbohydrate substrates ready for glycosidic bond synthesis.

Sugar or carbohydrate synthesis is important for the development of diagnostic tests, vaccines and new drugs. Conventional chemical synthesis in the laboratory is usually expensive and cumbersome; therefore great efforts are being made to use enzymes, which are natural catalysts. In this work we modified a robust glycosidase enzyme, which normally degrades carbohydrates, to do the opposite and synthetize carbohydrates. The modification consists on a single mutation of one active site amino acid. The main novelty of the work is that the engineered enzyme operates via a reaction mechanism (named *front-face* or *S_Ni-like*) that had not been previously observed in glycosidases, opening new possibilities for carbohydrate synthesis. Molecular biology techniques, together with the modeling of the reaction mechanism using a combination of molecular dynamics and quantum mechanics methods, have unraveled the new enzyme catalytic mechanism.

Ionization and Conformational Equilibria of Citric Acid: Delocalized Proton Binding in Solution

S. Madurga, M. Nedyalkova, F. Mas, J. L. Garcés.

J. Phys. Chem. A, *121* (2017) 5894.



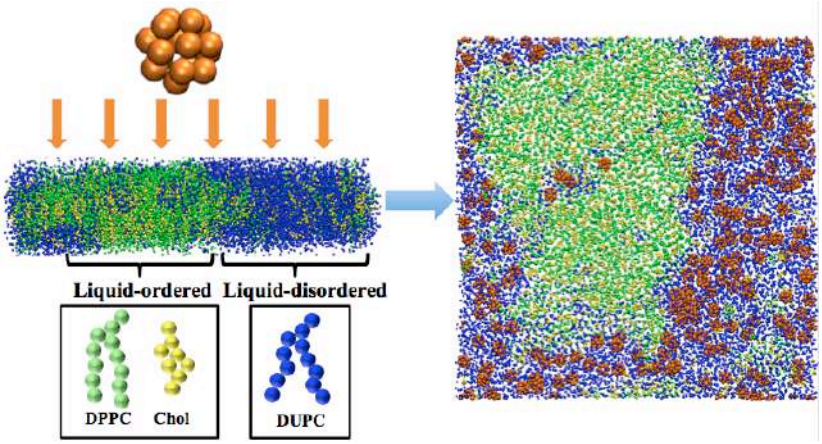
Calculation of localized and delocalized hydrogen bonds in the citric acid molecule.

The microspeciation of citric acid is studied by analyzing NMR titration data using *ab initio* and statistical mechanics techniques (site binding models). With this aim, *ab initio* MP2 calculations using the SMD polarizable continuum model for the solvent were performed and the fully roto-microspeciation of citric acid was elucidated. The results reveal that the exchange of the proton through the hydrogen bonds is in some cases produced without energetic barrier. This effect is specially relevant in the di-ionized form, with all the most stable conformations forming a Short, Strong, Low barrier (SSLB) hydrogen bond, which together would constitute the only microstate detected by NMR.

Effects of Fullerene on lipid bilayers displaying different liquid ordering: a coarse-grained molecular dynamics study

J. Sastre, I. Mannelli, R. Reigada.

Biochim. Biophys. Acta - General Subjects, *1861* (2017) 2872.



Our simulations show that segregating lipid membranes accumulate fullerene molecules in liquid-disordered domains. This behavior may have important consequences on the activity of biological membranes and on the bioconcentration of fullerene in living organisms.

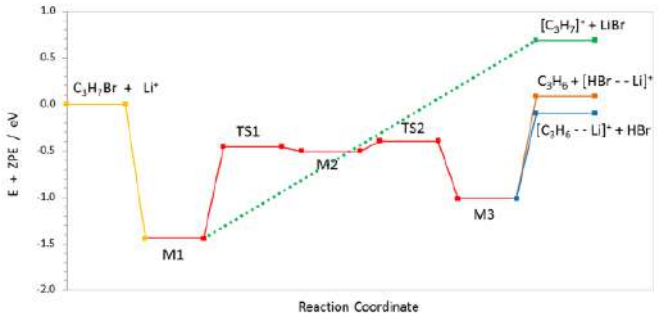
The toxic effects and environmental impact of nanomaterials, and in particular of Fullerene particles, are matters of serious concern. We report on a systematic coarse-grained molecular dynamics study of the interaction of fullerene molecules with simple model cell membranes. Addition of fullerene particles to phase-segregated ternary membranes is also investigated in the context of the lipid raft model for the organization of the cell membrane. Fullerene addition to lipid membranes modifies their structural properties like thickness, area and internal ordering of the lipid species, as well as dynamical aspects such as molecular diffusion and cholesterol flip-flop. Interestingly, we show that phase-segregating ternary lipid membranes accumulate fullerene molecules preferentially in the liquid-disordered domains, and this may have important consequences on the activity of biological cell membranes and on the bioconcentration of fullerene in living organisms.

LINE 4. REACTIVITY AND REACTIONS DYNAMICS

The role of Li^+ ions in the gas phase dehydrohalogenation and dehydration reactions of *i*-C_3H_7Br and *i*-C_3H_7OH molecules studied by radiofrequency-guided ion beam techniques and *ab initio* methods

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

J. Chem. Phys., *146* (2017) 134301.



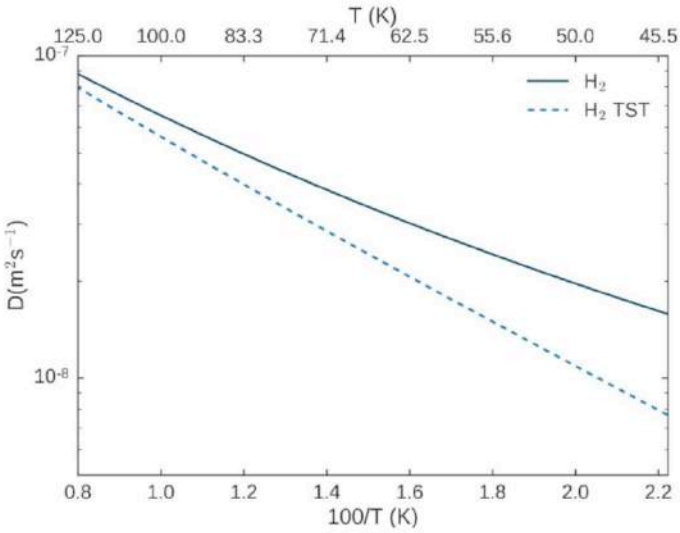
Schematic profile of the zero point energies of the different stationary points (minima and transition states) characterized along the reaction path calculated at the *ab initio* MP2 level on the singlet ground state of the Li^+ + *i*-C_3H_7Br. Energies of the minima (M) and transition states (TS) on the PES are referred to reactants and the connectivity among them is shown using the IRC method.

Elimination reactions play a relevant role in the preparation of unsaturated hydrocarbons and in gas phase alkali ions show an enhanced reactivity against their passive in solutions systems. In this work the experimental elimination reactions of H_2O and HBr species under single collision conditions have been studied when ions Li+(^1S_o) ions collide with gas phase *i*-C_3H_7Br and *i*-C_3H_7OH both being in their electronic state. Using a radiofrequency-guided ion beam (RF-GIB) technique the reaction products have been characterized by mass spectrometry. Experiments were done in the 0.010 - 10.00 eV center of mass energy range. For these reactive systems spectrometry mass analysis has shown the formation of $[C_3H_6$–Li$]^+$, [HBr-Li]$^+$, [H_2O-Li]+, $C_3H_7^+$ and the transitory adduct [Na - *i*-$C_3H_7Br]^+$. For all characterized products the corresponding excitation functions in absolute units were obtained allowing to calculate the corresponding formation reaction rate constants at 303.2 K. *Ab initio* structure calculations at the MP2 level relevant information on potential energy surfaces (PES) where elimination and decomposition reactions evolve adiabatically, characterizing different minima and transition state connected along the IRC. Topology features of the PES allow a qualitative interpretation of the experimental data and show the role of the lithium ion as a catalyst in elimination reactions.

Quantum dynamics of H_2 in a carbon nanotube: Separation of time scales and resonance enhanced tunneling

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

J. Chem. Phys., *147* (2017) 084103.



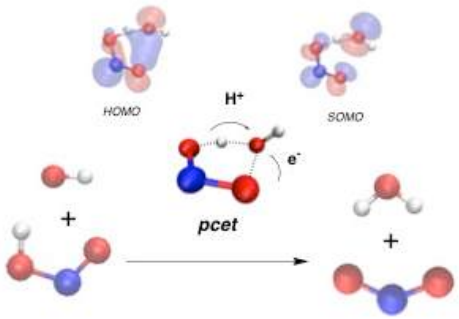
Diffusion rates for H_2 in a (8,0) carbon nanotube computed with TST (dotted line) and flux correlation functions (solid line).

We study the diffusion of H_2 in a narrow (8,0) carbon nanotube in the low pressure limit using quantum dynamics tools. Transmission coefficients for the elementary step of the transport process are calculated using the flux correlation function approach and diffusion rates are obtained using the single hopping model. We take advantage of the different time scales associated with the motion in the confined coordinates and the motion along the nanotube's axis to develop an exact diabatic representation. An adiabatic approximation on the system, separating the dynamics of confined and unbound coordinates, agrees almost perfectly with the numerically exact simulation. Using it we study the dynamics up to 20 ps. Resonance enhanced tunnelling is found to be the dominant transport mechanism at low energies, increasing the diffusion rate at T<120 K.

The Atmospheric Oxidation of HONO by OH, Cl, and ClO Radicals

J. M. Anglada, A. Solé.

J. Phys. Chem. A *121* (2017) 9698.

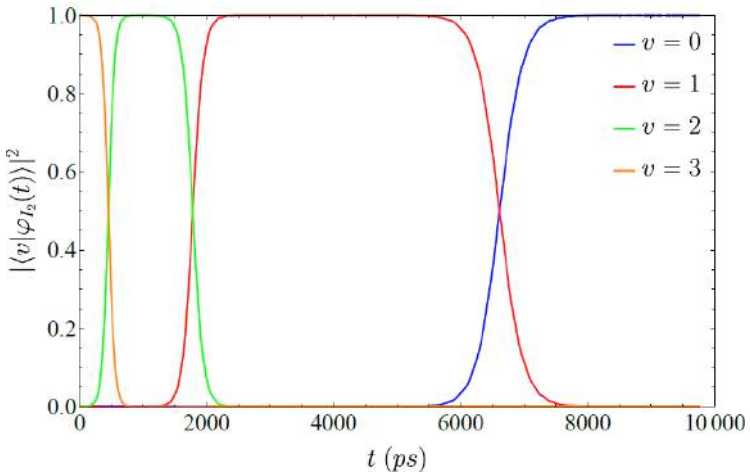


The atmospheric oxidation of nitrous acid by hydroxyl radical, chlorine atom and chlorine monoxide radical was investigated with high-level theoretical methods. Nitrous acid has two conformers (*cis* and *trans*) and we found a reaction path for the oxidation of each of these conformers with the radicals considered. In all cases, the oxidation of the *cis* conformer is much more favorable than the oxidation of the *trans* conformer. Interestingly all transition states in these oxidation processes follow a proton coupled electron transfer mechanism. Our computed rate constant at 298 K for the reaction of *cis*-HONO + •OH is 4.83 x 10^{-12} cm^3 $molecule^{-1}$ s^{-1}, in excellent agreement with their experimental values (4.85 x 10^{-12} and 6.48 x 10^{-12} cm^3 $molecule^{-1}$ s^{-1}). For the trans-HONO + •OH reaction our calculated rate constant at 298 K is 9.05 x 10^{-18} cm^3 $molecule^{-1}$ s^{-1}, and we computed an effective rate constant for the oxidation of the whole nitrous acid by hydroxyl radical of 1.81 x 10^{-12} cm^3 $molecule^{-1}$ s^{-1}. For the oxidation of nitrous acid by chlorine atom we predict greater rate constants (7.38 x 10^{-11}, 3.33 x 10^{-15}, and 2.76 x 10^{-11} cm^3 $molecule^{-1}$ s^{-1}, for the *cis* and *trans* conformers and for the whole HONO), these results suggesting that this reaction should contribute to the tropospheric oxidation of nitrous acid, especially in marine boundary areas, and to the formation of tropospheric ozone. For the oxidation of nitrous acid by chlorine monoxide we predict rate constants roughly 6 orders of magnitude smaller than the oxidation by chlorine atom, and therefore we consider that this process should play a minor role in the troposphere.

Vibrational energy relaxation dynamics of diatomic molecules inside superfluid helium nanodroplets. The case of the I_2 molecule

A. Vilà, M. Paniagua, M. González.

Phys. Chem. Chem. Phys. doi: 10.1039/c7cp05694j



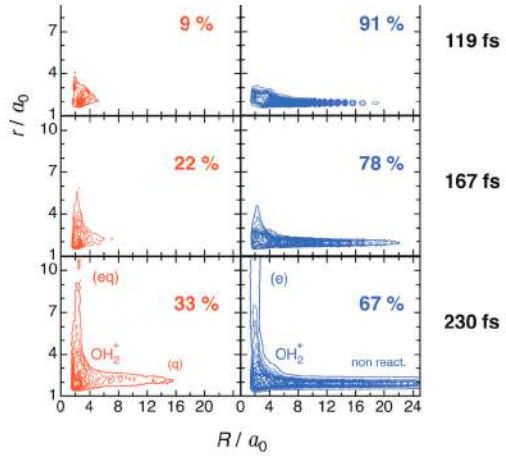
Time evolution of the vibrational populations for the initial excitation of the I_2 molecule to v=3.

The vibrational energy relaxation (VER) of a X_2 molecule in a ^4He superfluid nanodroplet (HeND; T = 0.37 K) was studied adapting a hybrid quantum approach proposed by us. In the first application the I_2 molecule was examined and this corresponds to the first theoretical investigation on VER of molecules embedded in HeND. The global relaxation from the initial excited state v down to the ground state (v = 0) happens in the ns scale and VER occurs following a cascade mechanism, where an arbitrary relaxation, e.g., v-1 → v-2, can only occur once the previous one has taken place. This mechanism was understood once the values of the coupling matrix elements were analyzed, and the time evolution of the populations of two consecutive vibrational levels was adequately described using a non-linear two-state Hamiltonian model. We hope that this first theoretical work on molecular VER dynamics in HeND will encourage researchers to investigate this important process about which we still know very little.

Nonadiabatic Renner-Teller quantum Dynamics of OH($X^2\Pi$) + H^+ reactive collisions

P. Gamallo, S. Akpinar, P. Defazio, C. Petrongolo.

Phys. Chem. Chem. Phys., *19* (2017) 4454.



wave packet density at three physical times over the ground potential energy surface X^1A'' (red) and first excited A^1A' (blue) at $\boldsymbol{J}$ = 10, p = + and K_0 = 0.

Nonadiabatic quantum dynamics study has been applied to $OH(X^2\Pi) + H'^+ \rightarrow OH'(X^2\Pi) + H^+$, exchange, $\rightarrow OH^+(X^3\Sigma^-) + H'(^2S)$, quenching, i $\rightarrow OH'^+ (X^3\Sigma^-) + H(^2S)$, exchange-quenching by means of time dependent real wave packet method and considering the Renner-Teller nonadiabatic couplings between both potential energy surfaces of OH_2^+ that correlate reactants with products, the ground one X^2A'' and the first excited A^2A'. We have obtained reactants state-specific probabilities, cross sections and rate constants along with the microscopic mechanism analysis. The results confirm that nonadiabatic channels, quenching and exchange-quenching, are the most reactive channels even more than the adiabatic channel of exchange, and that reactivity of quenching channels is similar, accounting for 97% to the total reactivity of the system.

III.2 PUBLICATION LIST

PUBLISHED ARTICLES

1. *Two-dimensional crystal CuS-electronic and structural properties.*
A. L. Soares Jr., E. C. dos Santos, A. Morales-Garcia, T. Heine, H. A. de Abreu, H. A. Duarte.
2D Mater., *4* (2017) 015041.

2. *Effective and highly selective CO generation from CO_2 using a polycrystalline α-Mo_2C catalyst.*
X. Liu, C. Kunkel, P. Ramírez de la Piscina, N. Homs, F. Viñes, F. Illas.
ACS Catalysis *7* (2017) 4323.

3. *Quantitative coordination-activity relations for the design of enhanced Pt catalysts for CO electro-oxidation.*
F. Calle-Vallejo, M. D. Pohl, A. S. Bandarenka.
ACS Catalysis *7* (2017) 4355.

4. *Structure- and coverage-sensitive mechanism of NO reduction on platinum electrodes.*
I. Katsonauros, M. C. Figueiredo, X. Chen, F. Calle-Vallejo, M. T. M. Koper.
ACS Catalysis *7* (2017) 4660.

5. *Accounting for bifurcating pathways in the screening for CO_2 reduction catalysts.*
F. Calle-Vallejo, M. T. M. Koper.
ACS Catalysis *7* (2017) 7346.

6. *1,6-Cyclophellitol cyclosulfates: a new class of irreversible glycosidase inhibitor.*
M. Artola, L. Wu, M. J. Ferraz, C.-L. Kuo, L. Raich, I. Z. Breen, W. A. Offen, J. D. C. Codée, G. A. van der Marel, C. Rovira, J. M. F. G. Aerts, G. J. Davies, H. S. Overkleeft.
ACS Centr. Sci., *3* (2017) 784–793.

7. *Precise probing of residue roles by post-translational β,γ-C,N aza-Michael mutagenesis in enzyme active sites.*
J. Dadová, K.-J. Wu, P. G. Isenegger, J. C. Errey, G. J. L. Bernardes, J. M. Chalker, L. Raich, C. Rovira, B. G. Davis.
ACS Centr. Sci., *3* (2017) 1168–1173.

8. *Redox-induced gating of the exchange interactions in a single organic diradical.*
R. Gaudenzi, J. De Bruijckere, D. Reta, I. d. P. R. Moreira, C. Rovira, J. Veciana, H. S. J. Van der Zant, E. Burzurí.
ACS Nano *11* (2017) 5879-5883.

9. *Iron oxide nanoparticles - in vivo/in vitro biomedical applications and in silico studies.*
M. Nedyalkova, B. Donkova, J. Romanova, G. Tzvetkov, S. Madurga, V. Simeonov.
Adv. Colloid Interface Sci., 249 (2017) 192-212.

10. *Spectroscopic observation of a hydrogenated CO dimer intermediate during CO reduction on Cu(100) electrodes.*
E. Pérez-Gallent, M. C. Figueiredo, F. Calle-Vallejo, M. T. M. Koper.
Angew. Chem. Int. Ed., *56* (2017) 3621.

11. *Zn-Zn double bonds, a theoretical study*.
J. Echeverría, A. Falceto, S. Alvarez.
Angew. Chem. Int. Ed., *56* (2017) 10151-10155.

12. *Nucleation of small silicon carbide dust clusters in AGB stars.*
D. Gobrecht, S. Cristallo, L. Piersanti, S. T. Bromley.
Astrophys. J., *840* (2017) 117.

13. *The catalase activity of catalase-peroxidases is modulated by changes in the pKa of the distal histidine.*
M. Machuqueiro, B. Victor, J. Switala, J. Villanueva, C. Rovira, I. Fita, P. C. Loewen.
Biochemistry *56* (2017) 2271–2281.

14. *Effects of fullerene on lipid bilayers displaying different liquid ordering: a coarse-grained molecular dynamics study.*
J. Sastre, I. Mannelli, R. Reigada.
Biochim. Biophys. Acta – General Subjects *1861* (2017) 2872-2882.

15. *Exploring the stability and reactivity of Ni_2P and Mo_2C catalysts using ab initio atomistic thermodynamics and conceptual DFT approaches.*
A. Morales-Garcia, J. He, P. Lyu, P. Nachtigall.
Biomass Conv. Bioref., *7* (2017) 377.

16. *Functionalization of γ-graphyne by transition metal adatoms.*
S. Kim, A. Ruiz Puigdollers, P. Gamallo, F. Viñes, J. Y. Lee.
Carbon *120* (2017) 63.

17. *DFT study of the role of N- and B-doping on structural, elastic and electronic properties of α-, β- and γ-graphyne.*
A. Ruiz-Puigdollers, P. Gamallo.
Carbon 114 (2017) 301.

18. *Carbon dissolution and segregation in platinum.*
P. Janthon, F. Viñes, J. Sirijaraense, J. Limtrakul, J. Y. Lee.
Catal. Sci. Technol., *7* (2017) 807.

19. *Oxide-based nanomaterials for fuel cell catalysis: the interplay between supported Pt atoms and particles.*
Y. Lykhach, A. Bruix, S. Fabris, V. Potin, I. Matolínová, V. Matolín, J. Libuda, K. M. Neyman.
Catal. Sci. Technol., *7* (2017) 4315-4345.

20. *Highly active Au/δ-MoC and Au/β-Mo_2C catalysts for the low-temperature water gas shift reaction: effects of the carbide metal/carbon ratio on the catalyst performance.*
S. Posada-Pérez, R. A. Gutiérrez, Z. Zuo, P. J. Ramírez, F. Viñes, P. Liu, F. Illas, J. A. Rodriguez.
Catal. Sci. Technol., *7* (2017) 5332.

21. *Surface composition changes of CuNi-ZrO_2 catalysts during methane decomposition: an operando NAP-XPS and density functional study.*
A. Wolfbeisser, G. Kovács, S. M. Kozlov, K. Föttinger, J. Bernardi, B. Klötzer, K. M. Neyman, G. Rupprechter.
Catal. Today *283* (2017) 134-143.

22. *Conformational analysis of the mannosidase inhibitor kifunensine: a quantum mechanical and structural approach.*
A. Males, L. Raich, S. J. Williams, C. Rovira, G. J. Davies.
ChemBioChem *18* (2017) 1496–1501.

23. *A new type of scaling relations to assess the accuracy of computational predictions of catalytic activities applied to the oxygen evolution reaction.*
L. G. V. Briquet, M. Sarwar, J. Mugo, G. Jones, F. Calle-Vallejo.
ChemCatChem *9* (2017) 1261.

24. *Investigation of easy-plane magnetic anisotropy in P-ligand square-pyramidal Co^{II} single ion magnets.*
K. Mondal, J. Jover, E. Ruiz, S. Konar.
Chem. Commun., *53* (2017) 5338-5341.

25. *An atypical interaction explains the high-affinity of a non-hydrolyzable S-linked 1,6-α-mannanase inhibitor.*
T. Belz, Y. Jin, J. Coines, C. Rovira, G. J. Davies, S. J. Williams**.**
Chem. Commun., *3* (2017) 9238–9241.

26. *Effect of second-order spin-orbit coupling on the interaction between spin states in spin-crossover systems.*
C. Sousa, A. Domingo, C. de Graaf.
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R. Martínez, M. Paniagua, J. Mayneris-Perxachs, P. Gamallo, M. González.
Phys. Chem. Chem. Phys., *19* (2017) 3857.

124. *Nonadiabatic Renner-Teller quantum dynamics of OH($X^2\Pi$) + H^+ reactive collisions.*
P. Gamallo, S. Akpinar, P. Defazio, C. Petrongolo.
Phys. Chem. Chem. Phys., *19* (2017) 4454.

125. *ZnO powders as multi-facet single crystals.*
F. Haque, S. Chenot, F. Viñes, F. Illas, S. Stankic, J. Jupille.
Phys. Chem. Chem. Phys., *19* (2017) 10622.

126. *Mercurophilic interactions: a theoretical study on the importance of ligands.*
J. Echeverría, J. Cirera, S. Alvarez.
Phys. Chem. Chem. Phys., *19* (2017) 11645-11654.

127. *Methanol–methanol and methanol–water systems: the intermolecular interactions controlling the transition from small clusters to the liquid phase.*
M. Albertí, A. Amat, A. Aguilar; F. Pirani.
Phys. Chem. Chem. Phys., *19* (2017) 16765.

128. *B-DNA model systems in non-terran bio-solvents: implications for structure, stability and replication.*
T. A. Hamlin, J. Poater, C. Fonseca Guerra, F. M. Bickelhaupt.
Phys. Chem. Chem. Phys., *19* (2017) 16969-16978.

129. *Approaching complexity of alkyl hydrogenation on Pd by density functional modelling.*
H. A. Aleksandrov, S. M. Kozlov, G. N. Vayssilov, K. M. Neyman.
Phys. Chem. Chem. Phys., *19* (2017) 21514-21521.

130. *Metal-doped ceria nanoparticles: stability and redox processes.*
A. Figueroba, A. Bruix, G. Kovács, K. M. Neyman.
Phys. Chem. Chem. Phys., *19* (2017) 21729-21738.

131. *Calix[: N] arene-based polyradicals: enhancing ferromagnetism by avoiding edge effects.*
D. Reta, I. d. P. R. Moreira, F. Illas.
Phys. Chem. Chem. Phys., *19* (2017) 24264-24270.

132. *Bandgap engineering by cationic disorder: case study on $AgBiS_2$.*
F. Viñes, G. Konstantatos, F. Illas.
Phys. Chem. Chem. Phys., *19* (2017) 27940.

133. *Fine tuning of optical transition energy of twisted bilayer graphene via interlayer distance modulation.*
E. del Corro, M. Peña-Alvarez, A. Morales-Garcia, M. Bousa, M. Mračko, R. Kolman, B. Pacakova, L. Kavan, M. Kalbac, O. Frank.
Phys. Rev B *95* (2017) 085138.

134. *ZrO_2 nanoparticles: a density functional theory study of structure, properties and reactivity.*
A. Ruiz Puigdollers, F. Illas, G. Pacchioni.
Rend. Lincei Sci. Fis. Nat., *28* (2017) 19.

135. *Continuous symmetry measures: a new tool in quantum chemistry.*
P. Alemany, D. Casanova, S. Alvarez, C. Dryzun, D. Avnir.
Rev. Comput. Chem., *30* (2017) 289-352.

136. *'Aggregation induced emission' active iridium(III) complexes with applications in mitochondrial staining.*
P. Alam, S. Dash, C. Climent, G. Kaur, A. R. Choudhury, D. Casanova, P. Alemany, R. Choudhury, I. R. Laskar.
RSC Adv., *7* (2017) 5642-5648.

137. *Structural properties, Judd – Ofelt calculations, and near infrared to visible photon up-conversion in Er^{3+}/Yb^{3+}/doped $BaTiO_3$ phosphors under excitation at 1500 nm.*
M. Vega, J. Llanos, P. Alemany, I. R. Martin.
RSC Adv., *7* (2017) 10529-10538.

138. *Study of the E–Z stilbene isomerisation in perchlorotriphenyl-methane (PTM) derivatives.*
F. Bejarano, I. Alcon, N. Crivillers, M. Mas-Torrent, S. T. Bromley, J. Veciana, C. Rovira.
RSC Adv., *7* (2017) 15278-15283.

139. *Direct covalent grafting of an organic radical core on gold and silver.*
M. R. Ajayakumar, I. Alcon, S. T. Bromley, J. Veciana, C. Rovira, M. Mas-Torrent.
RSC Adv., *7* (2017) 20076-20083.

140. *Measuring the spin-polarization power of a single chiral molecule.*
C. Aragonès, E. Medina, M. Ferrer-Huerta, N. Gimeno, M. Teixidó, J. L. Palma, N. Tao, J. M. Ugalde, E. Giralt, I. Díez-Pérez, V. Mujica.
Small *13* (2017) 1602519.

141. *Differential electrochemical conductance imaging at the nanoscale.*
M. López-Martínez, J. M. Artés, V. Sarasso, M. Carminati, I. Díez-Pérez, F. Sanz, P. Gorostiza.
Small *13* (2017) 1700958.

142. *Adsorption and dissociation of molecular hydrogen on orthorhombic β-Mo_2C and cubic δ-MoC (001) surfaces.*
S. Posada-Pérez, F. Viñes, R. Valero, J. A. Rodriguez, F. Illas.
Surf. Sci., *656* (2017) 24-32.

143. *Cohesion and coordination effects on transition metal surface energies.*
J. Ruvireta, L. Vega, F. Viñes.
Surf. Sci., *664* (2017) 45.

144. *Substrate-Controlled Aldol Reactions from α-hydroxy ketones.*
G. Aullón, P. Romea, F. Urpí.
Synthesis *49* (2017) 484-503.

145. *Substrate-mediated single-atom isolation: dispersion of Ni and La on γ-graphyne.*
S. Kim, P. Gamallo, F. Viñes, J. Y. Lee, F. Illas.
Theor. Chem. Acc., *136* (2017) 80.

146. *Modelization of the H_2 adsorption on graphene and molecular dynamics simulation.*
N. Faginas-Lago, Md Bin Yeamin, J. Sánchez Marín, I. G. Cuesta, M. Albertí, A. Sánchez de Merás.
Theor. Chem. Acc., *136* (2017) 91.

147. *Atomic ordering and Sn segregation in Pt-Sn nanoalloys supported on CeO_2 thin films.*
A. Neitzel, G. Kovács, Y. Lykhach, S. M. Kozlov, N. Tsud, T. Skála, M. Vorokhta, V. Matolín, K. M. Neyman, J. Libuda.
Top. Catal., *60* (2017) 522-532.

BOOK CHAPTERS AND PROCEEDINGS

1. *De dones, homes i molècules. Notes d'història, art i literatura de la química.*
   S. Alvarez.
   Edicions UB, Barcelona (2017), ISBN 978-84-475-3982-6.

2. *2.Diarylplatinum(II) scaffolds for kinetics and-mechanistic studies on the formation of platinacycles via an oxidative addition/reductive elimination/oxidative addition sequence.*
   G. Aullón, M. Crespo, J. Jover, M. Martínez.
   Adv. Inorg. Chem., edited by R. van Eldik and C. D. Hubbard, 70, chapter 6, 195-242, Elsevier (2017).

3. *Intermolecular interactions in crystals. Fundamentals of crystal engineering.*
   edited by J. J. Novoa, Royal Society of Chemistry, United Kingdom (2017).

4. *An application of the maximum principle in chemistry: a method to locate transition states.*
   J.M. Bofill, W. Quapp.
   Theoretical and Quantum Chemistry at the Dawn of the 21st Century edited by Ramon Carbó-Dorca and Tanmoy Chakraborty, Apple Academic Press Inc., USA (2017).

5. M*odelling enzymatic reaction-diffusion processes in in vivo-like systems.*
   P. M. Blanco, S. Madurga; J. L. Garcés; M. Cascante, F. Mas.
   Biology for Physics: Is there New Physics in Living Matter? European Physical Society Ed., ISBN: 979-10-96389-03-2, 20 (2017).

6. *Silicate nanoclusters: understanding their cosmic relevance from bottom-up modelling.*
   S. T. Bromley.
   Clusters: Structure, Bonding and Reactivity edited by M. T. Nguyen and B. Kiran, Springer, Switzerland (2017).

7. *Pharmaceuticals removal from water effluents by adsorption in activated carbons using Monte Carlo simulations.*
   D. Bahamon, L. F. Vega.
   27th European Symposium on Computer Aided Process Engineering edited by Antonio Espuña, Moisès Graells and Luis Puigjaner, Elsevier, Netherlands (2017).

III.3 OTHER ACTIVITIES

DOCTORALS THESES 2017

1. *Ligandos supramoleculares en complejos metálicos con propiedades físicas relevantes.*
   Lindley Maxwell Villacorta
   Supervisor/s: E. Ruiz.
   June 2017.

2. *Bioengineering single-protein wires.*
   Marta Pozuelo Ruiz
   Supervisor/s: I. Díez.
   July 2017.

3. *Theoretical study of excited states in molecules and molecular aggregates relevant for optoelectronic applications.*
   Clàudia Climent Biescas
   Supervisor/s: D. Casanova i P. Alemany.
   July 2017.

4. *Density functional modelling of materials for fuel cell catalysts with reduced content of critical components.*
   Alberto Figueroba Sanchez
   Supervisor/s: K. Neyman.
   July 2017.

5. *Field-effects on single molecular circuitry. Electronic transport from synthetic to biological models.*
   Albert Cortijos Aragones
   Supervisor/s: F. Sanz i I. Díez.
   July 2017.

6. *Conformational and mechanistic analyses of α- and β-glycosidase substrates by ab initio QM/MM methods.*
   Santiago Alonso Gil
   Supervisor/s: C. Rovira
   July 2017.

7. *Electrochemical tunneling microscopy and spectroscopy of electron transfer proteins.*
   Montse López Martinez
   Supervisor/s: I. Díez.
   September 2017.

8. *Desenvolupament de models per nanopartícules de TiO_2 i ZnO en fotocatàlisis.*
Oriol Lamiel Garcia
Supervisor/s: S. Bromley i F. Illas.
September 2017.

9. *New strategies of inhibition of K-Ras and study of the K-Ras/CaM interaction.*
Eduardo Garrido Sagarzazu
Supervisor/s: J. Rubio.
September 2017.

MASTERS THESES 2017

1. *Graphene Interaction with Ni(111): Description by Modern Dispersive Forces Approaches.*
Helena Muñoz Galán
Supervisor/s: F. Viñes
Master in nano-Science and nano-Technology.
Faculty of Chemistry, University of Barcelona.
February 2017.

2. *Elucidating the mechanisms of phase transitions in switchable biradical-based magnetic materials.*
Julia Schmidt
Supervisor/s: J. J. Novoa.
MSci Chemistry with Spanish for Science.
Imperial College London.
June 2017.

3. *Computational study of enzyme-substrate interactions in galactosyltranferases.*
David Almacellas Salillas
Supervisor/s: C. Rovira
Master in Organic Chemistry.
Faculty of Chemistry, University of Barcelona.
July 2017.

4. *Modelling the Michaelis complex of CtCel124 glycosyl hydrolase.*
Albert Pla Mas
Supervisor/s: C. Rovira.
Master in Atomistic and Multiscale Computational Modelling in Physics, Chemistry and Biochemistry.
Faculty of Chemistry, University of Barcelona.
July 2017.

5. *On the Accuracy of Density Functionals in Describing Transition Metal Surface Properties.*
Lorena Vega Domínguez
Supervisor/s: F. Viñes.
Master in Atomistic and Multiscale Computational Modelling in Physics, Chemistry and Biochemistry.
Faculty of Chemistry, University of Barcelona.
July 2017.

6. *Pressure and temperature effects on the symmetry of the atomic coordination environment in tetrahedral solids.*
Xavier Marugan Ferrer
Supervisor/s: P. Alemany
Master in Atomistic and Multiscale Computational Modelling in Physics, Chemistry and Biochemistry.
Faculty of Chemistry, University of Barcelona.
July 2017.

7. *Theoretical and Computational Study of Sulfur Compounds Reactivity in Prebiotic Chemistry: The Whitesides Network of Thiols and Thioesters.*
João Miguel dos Santos Nicolau Inês
Supervisor/s: I. de P. R. Moreira, J. M. Bofill
Master in Atomistic and Multiscale Computational Modelling in Physics, Chemistry and Biochemistry.
Faculty of Chemistry, University of Barcelona.
September 2017.

8. *On-Lattice Monte Carlo simulation of enzyme kinetics in crowded intracellular environments.*
Enric Fortín Foz
Supervisor/s: F. Mas.
Master in Atomistic and Multiscale Computational Modelling in Physics, Chemistry and Biochemistry.
Faculty of Chemistry, University of Barcelona.
September 2017.

9. *Modeling enzymatic reaction-diffusion processes in crowded media by Brownian Dynamics simulations.*
Marí López Berbel
Supervisor/s: F. Mas.
Master in Atomistic and Multiscale Computational Modelling in Physics, Chemistry and Biochemistry.
Faculty of Chemistry, University of Barcelona.
September 2017.

SCIENTIFIC CONFERENCES AND MEETINGS 2017

1st Biology for Physics: Is there Any Physics in Living Matter?
Barcelona (Spain), 15-18 January 2017

Modelling enzymatic reaction-diffusion processes in in vivo-like systems (poster)
P. M. Blanco, S. Madurga, J. L. Garcés, M. Cascante, F. Mas

Dissecting the roles of the aberrant collagen mechanobiology in lung fibrosis and cancer (poster)
R. Ikemori, M. Gabasa, M. Puig, A. Giménez, R. Galgoczy, I. Pastor, F. Mas, N. Reguart, A. Vaubet, A. Labernardie, X. Trepat, J. Alcaraz

CM1401 COST Meeting: Our Astrochemical History Week
Faro (Portugal), 16-20 January 2017

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

MOLESCO Molecular Scale Electronics (3rd Annual Meeting and Workshop)
Granada (Spain), 17-21 January 2017

Transport in biological motifs and metalloproteins (invited talk)
I. Díez-Pérez, M. Ruiz

The eSSENCE of . . . Computational Chemistry & Physics, CECAM program seminar series
Uppsala (Sweden), 26 January 2017

Modelling catalytic nanomaterials - as simple as possible, but not simpler (invited talk)
K. M. Neyman

II Workshop on Chemistry of Group 11 Elements
Barcelona (Spain), 26-27 January 2017

G. Aullón *(organizing committee)*

Trinuclear gold-carborane as a host structure (poster)
G. Aullón, J. M. Oliva, A. Laguna

Can DFT accurately reproduce reaction yields? A computational study of copper-mediated pentafluoroethylation of benzoic acid chlorides (*poster*)
J. Jover

The eSSENCE of . . . Computational Chemistry & Physics, CECAM program seminar series
Stockholm (Sweden), 27 January 2017

Modelling catalytic nanomaterials - as simple as possible, but not simpler (invited talk)
K. M. Neyman

8th European Symposium on Computing π-conjugated Compounds (CπC)
Málaga (Spain), 27-28 January 2017

Influence of the sulfur bridge in the photophysics of covalent naphthalene dimers (oral communication)
C. Climent

funCOS seminar series
Erlangen (Germany), 30 January 2017

Effect of ionic Pt on the reducibility of Pt/CeO_2 nanocomposites (invited talk)
K. M. Neyman

5th International Conference on Water, Energy & Environment (ICWEE/5)
Abu Dhabi (United Arab Emirates), 28 February – 2 March 2017

Modeling pharmaceuticals removal from water effluents by adsorption in activated carbons (oral communication)
L. F. Vega, D. Bahamon

BCA Spring Meeting
Lancaster (United Kingdom),11 April 2017

Transition metal coordination polyhedra: shape, spin and secondary bonding (Plenary lecture)
S. Alvarez

International Conference on Multifunctional, hybrid and nanomaterials
Lisbon (Portugal), 6-10 March 2017

Antimicrobial and biofilm preventing functionalized optical surfaces (poster)
M. A. Noyan, R. Sibilo, I. Mannelli, R. Reigada, M. Mazumder, M. Lakadamyali, V. Pruneri

Department colloquium
Upton (USA), 20 March 2017

Computational design of bimetallic nanocrystals (invited talk)
K. M. Neyman

Advances in computational and experimental studies of solids: Richard Catlow 70th meeting
Oxford (United Kingdom), 10-12 April 2017

Size dependent transitions in nano-oxides (oral communication)
S. T. Bromley

12th Carbohydrate Bioengineering Meeting (CBM12)
Vienna (Austria), 23-26 April 2017

A front-face mechanism 'synthase' engineered from a retaining hydrolase. Mechanistic insight from QM/MM metadynamics (invited talk)
C. Rovira

CNRS
Toulouse (France), 5 May 2017

Magnetic transition metal complexes: from single-molecule magnets to magnetoresistance single-molecule devices (oral communication)
E. Ruiz

10th European School on Molecular Nanoscience (ESMOLNA)
San Lorenzo del Escorial (Spain), 7-12 May 2017

Ferrocene: Old molecule with new relevant physical properties (invited talk)
E. Ruiz

Aportando valor al CO_2
Tarragona (Spain), 9-10 May 2017

Finding the optimum cation content in faujasites for post-combustion CO_2 capture in swing adsorption processes (oral communication)
D. Bahamon, H. Prats, G. Alonso, X. Giménez, P. Gamallo, R. Sayós

Hybrid Quantum Mechanics / Molecular Mechanics (QM/MM) Approaches to Biochemistry and beyond / CECAM-MARVEL QM/MM School
Lausanne (Switzerland), 15-19 May 2017

C. Rovira *(organizing committee)*

The reaction intermediate of GH18 chitinases: substrate conformation and protonation state (poster)
J. Coines, M. Alfonso-Prieto, X. Biarnés, A. Planas, C. Rovira

Catalytic study of β-galactocerebrosidase (poster)
A. Nin-Hill, Ll. Raich, C. Rovira

Master Química XIII
Barcelona (Spain), 17 May 2017

Estudi de l'efecte del crowding macromolecular emprant simulacions de dinàmica browniana (poster)
M. López, P. M. Blanco, F. Mas, S. Madurga

III Russian Congress on Catalysis "Roskataliz-2017"
Nizhny Novgorod (Rusia), 22-26 May 2017

K. M. Neyman *(chairman in scientific session)*

Computational engineering of bimetallic catalysts to speed-up their targeted manufacturing (invited talk)
K. M. Neyman

European Workshop on Theoretical approaches of Molecular Magnetism: Jujols IX,
Tortosa (Spain), 22-26 May 2017

Modeling the ligand tuning effect over the transition temperature in spin-crossover systems using density functional methods (invited talk)
E. Ruiz

Magnetic Fingerprint of Planar Bistable Molecule-Based Magnets (oral communication)
T. Francese

Cicle Elements de Química a la Literatura, CSIC
Barcelona (Spain), 30 May 2017

La química en la literatura: de cites breus a cosmogonies (invited talk)
S. Alvarez

Máster Oficial Química de Materials Aplicada de la Universitat of Barcelona
Barcelona (Spain), 2 June 2017

G. Aullón *(coordinator)*

8th IQTCUB Symposyum
Barcelona (Spain), 2 June 2017

J. Cirera, M. Deumal *(organizing committee)*

Cerca del contingut de cations òptim en faujasites per a la captura de CO_2 de post-combustió amb processos d'adsorció tipus swing (poster)
D. Bahamon, H. Prats, G. Alonso, X. Giménez, P. Gamallo, R. Sayós

Effect of the pressure on the synthesis of ADOR zeolites (oral communication)
A. Morales-Garcia

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

Study of the effect of macromolecular crowding with brownian dynamics simulations (poster)
M. López, P. M. Blanco, F. Mas, S. Madurga

Realistic modelling of the nucleation of nanosilicate dust particles using atomistic simulations (poster)
A. Macià, S. T. Bromley

BCC transition metal surfaces: trends in work functions and surface energies (poster)
L. Vega, F. Viñes

On-lattice Monte Carlo simulations of enzyme kinetics in crowded intracellular environments (poster)
E. Fortín, S. Madurga, E. Vilaseca, F. Mas

Study of the effect of macromolecular crowding with brownian dynamics simulations (poster)
M. López, P. M. Blanco, F. Mas, S. Madurga

Towards a realistic modelling of protein diffusion in polymer crowded media (poster)
P. M. Blanco, S. Madurga, J. L. Garcés, F. Mas

Angular momentum effects on the Ne + $(^4He)_N \rightarrow Ne@(^4He)_{N'}$ + $(N\text{-}N')^4He$ capture process and quantised vortex formation: a quantum-classical approach (poster)
M. Blancafort, A. Vilà, M. González

Importance of the tunneling effect on the diffusion of H_2 along a carbon nanotube (oral communication)
M. Mondelo-Martell, F. Huarte-Larrañaga

Nanocosmos Interstellar Dust Meeting
Toulouse (France), 12-13 June 2017

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

1st ELECMI International Workshop
Zaragoza (Spain), 12-14 June 2017

Studying chemical reactions at the nanoscale (invited talk)
I. Díez-Pérez, A. C. Aragones, N. Darwish

4th Conference on Multiscale Modelling of Materials and Molecules
Uppsala (Sweden), 12-14 Juny 2017

Computational design of bimetallic nanocrystals (invited talk)
K. M. Neyman

Icmat 2017 - Materials Research Society of Singapore
Singapore (Singapore), 18-23 June 2017

Force Fields in single-molecule wires (invited talk)
I. Díez-Pérez, A. C. Aragones, N. Darwish

9th International Conference Engineering of Chemical Complexity (ECC9)
Vilanova i la Geltrú (Spain), 19-22 June 2017

R. Reigada *(organizing committee)*

Towards a realistic modelling of protein diffusion in polymer crowded media (poster)
P. M. Blanco, S. Madurga, J. L. Garcés, F. Mas

FemEx-Netherlands, Promoting female excellence in theoretical and computational chemistry
Putten (Netherlands), 22-25 June 2017

Spin states in Fe(II) materials (oral communication)
C. Sousa

XXXVI Reunión Bienal de la Real Sociedad Española de Química
Sitges (Spain), 25-29 June 2017

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

Interacciones intermoleculares en hidruros del grupo 13 (poster)
J. Echeverría, G. Aullón, S. Alvarez

Dihydrogen Interactions in group 14 Hydrides (poster)
G. Aullón, J. Echeverría, S. Alvarez

Re-thinking TTTA magnetism: moving from a static to a dynamical computational perspective (poster)
S. Vela, F. Mota, J. J. Novoa, J. Ribas-Ariño, M. Deumal

The complex mechanochemistry of disulfide bond reduction in alkaline solution (oral communication)
J. Ribas-Ariño

B-DNA stability and replication in non-terran biosolvents (oral communication)
J. Poater, T.A. Hamlin, C. F. Guerra, F. M. Bickelhaupt

Everyday analogies to understand difficult concepts: aromaticity (oral communication)
S. Simon, J. Poater, M. Duran, M. Solà

The Baird rule and the aromaticity of low-lying excited states (oral communication)
M. Solà, O. El-Bakouri, J. Poater, F. Feixas

CECAM meeting "Dopant dynamics in superfluid helium-4 nanodroplets: form statics to time dependent He-DFT"
Toulouse (France), 25-30 June 2017

Dynamics of chemical processes involving atoms/molecules and superfluid helium nanodroplets (oral communication)
A. Vilà, M. Blancafort, R. Mayol, M. González

Dynamics and kinetics of low temperature capture processes in Rg + H_2^+ collisions (oral communication)
M. P. Puyuelo, P. A. Enríquez, P. Gamallo, M. González

3rd BOOK-D (Bordeaux Olivier Kahn Discussions)
Bordeaux (France), 26-27 June 2017

Modelling spin-crossover with theoretical tools: Frommolecules to metal-organic frameworks (*invited talk*)
J. Cirera

Congreso de la Sociedad Española de Catálisis (SECAT17)
Oviedo (Spain), 26-28 June 2017

Deactivation of molybdenum carbide catalyst in the hydrodeoxygenation (HDO) of phenol by the presence of water (oral communication)
A. Morales-García, P. Lyu, J. Engelhardt, F. Schüth, P. Nachtigall

Au/MoC as an efficient catalyst for H_2 production: experiments and theoretical (oral communication)
S. Posada-Pérez, P.J. Ramírez, F. Viñes, J. A. Rodríguez, F. Illas

EuCheMS Inorganic Chemistry Conference (EICC-4)
Copenhagen (Denmark), 2-5 July 2017

Modelling the ligand fine tuning effect over the transition temperature in spin-crossover systems with density functional methods (oral communication)
J. Cirera

Can DFT accurately reproduce reaction yields? a computational study of copper-mediated pentafluoroethylation of benzoic acid chlorides (poster)
J. Jover

19th European Carbohydrate Symposium (EUROCARB)
Barcelona (Spain), 2-6 July 2017

Catalytic study of β-galactocerebrosidase (poster)
A. Nin-Hill, Ll. Raich, C. Rovira

Sugar conformational changes and reactivity of carbohydrate-active enzymes. Insight from QM/MM metadynamics simulations (invited talk)
C. Rovira

The reaction intermediate of GH18 chitinases: substrate conformation and protonation state (poster)
J. Coines, M. Alfonso-Prieto, X. Biarnés, A. Planas, C. Rovira

XIV International Workshop on Quantum Reactive Scattering
Trieste (Italy), 3-6 July 2017

The role of tunneling on the diffusion rate of H_2 and D_2 along a narrow SWCNT (keynote talk)
M. Mondelo-Martell, F. Huarte-Larrañaga

Quantum dynamics of H_2 in a carbon nanotube: timescale separation and resonance enhanced tunneling (keynote talk)
M. Mondelo-Martell, F. Huarte-Larrañaga

Frontiers of multi-scale modeling in materials, energy & catalysis III
Heiligenhafen (Germany), 3-7 July 2017

Optimal faujasite structures for post combustion CO_2 separation in swing adsorption processes: a computational study (oral communication)
H. Prats, D. Bahamón, G. Alonso, X. Giménez, P. Gamallo, R. Sayós

7th Iberian Meeting on Colloids and Interfaces (RICI7)
Madrid (Spain), 4-7 July 2017

Towards a realistic modelling of protein diffusion in polymer crowded media (poster)
P. M. Blanco, S. Madurga, J. L. Garcés, F. Mas

XXXIII Reunió de la xarxa de Referència en Química Teòrica i Computacional de Catalunya (XrQTC)
Tarragona (Spain), 5-6 July 2017

On-lattice Monte Carlo simulations of enzyme kinetics in crowded intracellular environments (poster)
E. Fortín, S. Madurga, E. Vilaseca, F. Mas

XXXVI Biennial Meeting of the Real Sociedad Española de Física
Santiago de Compostela (Spain), 17-21 July 2017

Hydrogen diffusion along SWCNTs: time-scale separation and tunneling effects (oral communication)
F. Huarte-Larrañaga, M. Mondelo-Martell

Hands-on Workshop Density-Functional Theory and Beyond: Accuracy, Efficiency and Reproducibility in Computational Materials Science
Humboldt University, Berlin (Germany), 31 July – 11 August 2017

First principles study of size, shape, and phase effects on ZnO photocatalyst nanostructures (poster)
F. Viñes, O. Lamiel-Garcia, S. T. Bromley, F. Illas

Swedish Theoretical Chemistry Conference 2017 – Bridging gaps
Gotemburg (Sweden), 16-18 August 2017

Density-functional modelling of ceria-based nanomaterials for catalysis and energy technologies (keynote talk)
K. M. Neyman

245th ACS National Meeting
Washington DC (United States), 20-24 August 2017

Could we make shorter Zn-Zn bonds? (invited talk)
S. Alvarez

Photophysics of naphthalene dimers controlled by the sulfur bridge oxidation (oral communication)
C. Climent

Effect of temperature on the symmetry of molecules and solids: a continuous symmetry measures study (invited talk)
P. Alemany

Computational modeling of catalytic metal/metal-oxide nanostructures (invited talk)
K. M. Neyman

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

Density-functional modeling of materials for single-atom catalysis based on nanostructured ceria (invited talk)
K. M. Neyman

Catalysis by natural and engineered glycosidases. An atomistic view from QM/MM simulations (invited talk)
C. Rovira

XIII European Congress on Catalysis (EuropaCat-2017)
Florence (Italy), 27-31 August 2017

Activation of oxygen in the ceria lattice by incorporation of platinum in Pt/CeO_2 catalysts for low-temperature CO oxidation (oral communication)
I. Boronin, A. I. Stadnichenko, E. M. Slavinskaya, T. Y. Kardash, V. V. Muravyov, A. Figueroba, A. Bruix, K. M. Neyman

How nanoscale metal-oxide boundaries activate micrometer-sized metal particles for CO oxidation via a long-range effect (oral communication)
Y. Suchorski, S. M. Kozlov, M. Datler, I. Bespalov, K. M. Neyman, G. Rupprechter

68th Annual Meeting of the International Society of Electrochemistry
Rhode Island (United States), 27 August – 1 September 2017

Single-molecule electrochemically-gated field-effect transistors (keynote talk)
I. Díez-Pérez, A. C. Aragonés, N. Darwish

33rd European Conference on Surface Science (ECOSS-33)
Szeged (Hungary), 27 August – 1 September 2017

Efficient computational engineering of bimetallic nanocrystals (invited talk)
K. M. Neyman, G. Kovács, S. M. Kozlov

Spectroscopy and microscopy of catalytic processes on well-defined surfaces: from UHV to operando conditions (invited talk)
G. Rupprechter, Y. Suchorski, S. M. Kozlov, M. Datler, I. Bespalov, K. M. Neyman

11th Triennial Cogress of the World Association of Theoretical and Computational Chemists (WATOC 2017)
Munich (Germany), 27 August - 1 September 2017

An algorithm to locate optimal bond breaking points on potential energy surfaces for mechanochemical reactions (poster)
J. M. Bofill, J. Ribas-Ariño, S. P. García, W. Quapp

Unraveling the magnetic transition temperature from changes in spin correlation (oral communication)
M. Deumal

Magnetic fingerprint of self-assembling DTA-based molecule-based magnets (oral communication)
T. Francese

Optimal Faujasite structures for post combustion CO_2 capture in swing adsorption processes (poster)
H. Prats, D. Bahamón, G. Alonso, X. Giménez, P. Gamallo, R. Sayós

Adsorption of post–combustion gases by Mg–MOF–74 (poster)
F. Keshavarz, O. Sánchez, D. Bahamon, P. Gamallo, X. Giménez, R. Sayós

69th Annual Meeting of the Electrochemical Society of Electrochemistry
Bologna (Italy), 2-7 September 2017

I. Díez-Pérez *(symposium 16 organizer: Micro- and Nano-Scale Platforms to Study Electron Transport in Bio/Molecular Systems: from Fundamentals to Molecular Devices)*

Modeling Interactions in Biomolecules VIII
Pilsen (Czech Republic), 3-8 Setembre 2017

How non-terran biosolvents affect the structure and stability of B-DNA (oral communication)
J. Poater, T. A. Hamlin, C. Fonseca Guerra, F. M. Bickelhaupt

MGMS international meeting: QM/MM Methods and Applications
Manchester (United Kingdom), 4-6 September 2017

Sugar conformational changes and catalytic mechanisms of carbohydrate-active enzymes (invited talk)
C. Rovira

11th European Conference on Theoretical and Computational Chemistry (EUCO 2017)
Barcelona (Spain), 4-7 September 2017

M. Deumal, R. Sayós *(organizing committee, chairmen and local committee members)*

Unraveling the magnetic transition temperature from changes in spin correlation (oral communication)
M. Deumal

Molecular dynamic simulations of oil-water wetting on mineral surfaces (oral communication)
G. Alonso, P. Gamallo, C. Rincón, R. Sayós

Ti(IV)-enolates can act as nucleophilic or birradical reagents: new reactivity induced by valence tautomerism (oral communication)
I. de P. R. Moreira, C. Heras, J. M. Bofill, A. Gómez-Palomino, P. Romea, F. Urpí

Conformationally induced paramagnetism in aryl substituted 2-imino-thiazole derivatives (poster)
C. Heras, R.Valero, G. Albareda, F. López-Calahorra, I. de P. R. Moreira, J. M. Bofill

Computational Advances in Drug Discovery - SBDD2017
Lausanne (Swisszertland), 5-8 September 2017

Sugar conformational changes and catalysis of carbohydrate-active enzymes (invited talk)
C. Rovira

6th Workshop of the European Doctorate in Theoretical Chemistry and Computational Modelling (TCCM – 2017)
Barcelona (Spain), 8 September 2017

On the calculation of interfacial tension and contact angle applied to rock/oil/water (oral communication)
G. Alonso, P. Gamallo, R. Sayós

Effect of Si/Al ratio on post combustion CO_2 capture by adsorption with faujasites (oral communication)
H. Prats, D. Bahamon, G. Alonso, X. Giménez, P. Gamallo, R. Sayós

Catalysts and catalysis through methods on models (oral communication)
F. Viñes, S. T. Bromley, K. M. Neyman, F. Illas

Models of magnesium silicate dust cores. Comparison of physical properties of different methods (oral communication)
A. Macià

Using open-shell molecules to design 2D covalent networks with controllable properties (oral communication)
I. Alcón

Highly-active Au/δ-MoC and Au/β-Mo_2C catalysts for the low-temperature water gas shift reaction (oral communication)
S. Posada-Pérez, R. A. Gutiérrez, Z. Zuo, P. J. Ramírez, F. Viñes, P. Liu, F. Illas, J. A. Rodriguez

International Workshop Advanced Materials 2017
Pomorie (Bulgaria), 10-13 September 2017

Catalysts and catalysis through methods on models (oral communication)
F. Viñes, S. T. Bromley, K. M. Neyman, F. Illas

On the accuracy of density functionals in describing transition metal surface properties (oral communication)
L. Vega, J. Ruvireta, F. Viñes, F. Illas

C poisoning on noble and Pt-group metals (oral communication)
O. Piqué, F. Viñes

CECAM Meeting - Big-Data driven Materials Science
Lausanne (Swisszertland), 11-13 September 2017

Learning how oxide materials evolve from nano to bulk (oral communication)
S. T. Bromley

Joint Iberian Meeting on Atomic and Molecular Physics (IBER 2017)
Barcelona (Spain), 12-14 September 2017

A. Aguilar *(organizing committee, chair)*
F. Huarte-Larrañaga *(organizing committee, secretary*)
M. Albertí, M. González, J. M. Lucas *(organizing committee)*

What can molecular simulations do for industrial processes? (oral communication)
P. Gamallo

Dynamics of the gas phase capture processes Rg + $H_2^+ \rightarrow RgH_2^+$ (Rg: He, Ne, Ar) (*poster*)
M. P. Puyuelo, P. A. Enríquez, P. Gamallo, M. González

Vibrational relaxation quantum dynamics of diatomic molecules inside superfluid helium nanodroplets. The case of I_2 (oral communication)
A. Vilà, M. Paniagua, M. González

Molecular photodissociation in superfluid helium nanodroplets. A quantum dynamics study of $Br_2(X) + h\nu \rightarrow Br_2(B) \rightarrow Br + Br^*$ (poster)
A. Vilà, M. González

Quantum-classical dynamics of the capture process of atoms by superfluid helium nanodroplets. The Ne + $(^4He)_{500}$ system and the influence of angular momentum (*poster*)
M. Blancafort, A. Vilà, M. González

Capture of Ne atoms by superfluid ^4He nanodroplets at low energy. Quantum vs classical comparison at J=0 (poster)
A. Sopena, A. Vilà, M. González

Transition from small clusters to neat methanol (poster)
M. Albertí, A. Amat, A. Aguilar, F. Pirani

Molecular hydrogen confined in carbon nanotubes: quantum dynamics calculations and resonance enhanced diffusion (poster)
M. Mondelo, F. Huarte-Larrañaga

The role of Li^+ ions in gas phase dehydrohalogenation and dehydration reactions of i-C_3H_7Br and i-C_3H_7OH molecules (poster)
E. López, J. M. Lucas, J. de Andrés, M. Albertí, J. M. Bofill, A. Aguilar

Non-adiabatic processes in $N_2O(X^1\Sigma^+)$ + $Na^+(^1S_0)$ gas phase collisions in the few keV energy range (poster)
J. M. Lucas, J. de Andrés, M. Albertí, J. M. Bofill, A. Aguilar

8th International Conference on Theory of Atomic & Molecular Clusters (TAMMC VIII)
Pekin (China), 17-22 September 2017

Properties of realistic models of semiconducting nanoparticles (invited talk)
F. Illas

In-silico engineering bimetallic nanocrystals (invited talk)
K. M. Neyman

10 th World Congress of Chemical Engineering (WCCE 2017)
Barcelona (Spain), 1-5 October 2017

Effect of Si/Al ratio in faujasites for post combustion CO_2 capture via pressure and temperature swing adsorption processes (oral communication)
D. Bahamon, H. Prats, G. Alonso, X. Giménez, P. Gamallo, R. Sayós

European Symposium on Computer-Aided Process Engineering, ESCAPE-27
Barcelona (Spain), 1-5 October 2017

Pharmaceuticals removal from water effluents by adsorption in activated carbons using Monte Carlo simulations (oral communication)
D. Bahamon, L. F. Vega

6th Jornades sobre l'Ensenyament de la Química a Catalunya (JEQC - 2017)
Expoquimia 2017, Barcelona (Spain), 2-6 October 2017

El Postdoc (oral communication)
F. Viñes

6th Mini-Workshop on Statistical and Molecular Biophysics
Trieste (Italy), 18-19 October 2017

Carbohydrate-active enzymes: sugar conformations and reactivity (invited talk)
C. Rovira

FEBS3 + 1st Joint Meeting of the French-Portuguese-Spanish Biochemical Molecular Biology Societies. XL SEBBM Congress
Barcelona (Spain), 23-26 October 2017

Metabolic characterization of castration-resistant prostate cancer (CRPC): Metabolic phenotype associated with metastatic progression (poster)
C. Balcells, I. Marín de Mas, M. Tarrado-Castellarnau, S. Marín, F. Mas, T. M. Thompson, M. Cascante

American Institute of Chemical Engineers (AIChE) 2017 Annual Meeting
Minneapolis (United States), 29 October – 3 November 2017

Understanding the removal of pharmaceuticals from water effluents by adsorption in activated carbons – a molecular simulation approach (oral communication)
L. F. Vega, D. Bahamon.

3rd International Conference "Electronic Structure Theory for Accelerated Materials Design: New Tool for Materials Science"
Moscou (Russia), 30-31 October 2017

Computational engineering of bimetallic nanocrystals (keynote talk)
K. M. Neyman

Theory seminars of the Institute for Solid State Physics of the University of Tokyo
Chiba (Japan), 31 October 2017

Spin transitions in spiro-biphenalenyl-based radicals: identification of the driving forces and the origin of bistability (oral communication)
J. Ribas-Ariño

EMN Meeting on Computation and Theory
Dubai (United Arab Emirates), 6-10 November 2017

Bridge between the aromaticity of polycyclic aromatic hydrocarbons and closo borohydrides (oral communication)
J. Poater, M. Solà, C. Viñas, F. Teixidor

International Conference on NANO- AND FUNCTIONAL MATERIALS: Interface between Science & Engineering (NFM-2017)
Rajasthan (India), 16-18 November 2017

Molecular modeling of organometallic Ir(III) compounds relevant for optoelectronic applications (invited talk)
P. Alemany

Symposium on the occasion of Paul Bagus' 80th Birthday
Berlin (Germany), 19 November 2017

Core level binding energies, Paul and me: a trip from HF and beyond to DFT and GW based methods (invited talk)
F. Illas

19th International Workshop on Nanoscience & Nanotechnology
Sofia (Bulgaria), 24-25 November 2017

Ionization and conformational equilibria of citric acid: delocalized proton binding in solution (oral communication)
M. Nedyalkova, S. Madurga, F. Mas, J. L. Garcés

A Model provides insight into electric field-induced rupture mechanism of water-in-toluene emulsion films (oral communication)
M. Nedyalkova, D. Diminova, S. Pisov, N. Panchev, S. Madurga, A. Proykova

The Boron oxide glasses and nanocomposites: synthetic, structural and statistical approach (oral communication)
H. Hristov, M. Nedyalkova, S. Madurga, V. Simeonov

18th European Meeting on Environmental Chemistry
Porto (Portugal), 26-29 November 2017

Computational & chemiinformatics approach to characterization of green solvents (poster)
M. Nedyalkova, M. Tobiszewski, S. Madurga, F. Pena-Pereira, V. Simeonov, J. Namiesnik

Computational Modeling of Materials School
Sofia (Bulgaria), 4-5 December 2017

Learning how oxide materials evolve from nano to bulk (oral communication)
S. T. Bromley

Modeling spin-crossover in condensed phase from molècules to metal-organic-frameworks (oral communication)
J. Cirera

Noncovalent interactions: a useful tool for crystal and materials design (oral communication)
J. Echeverría

Molecular dynamics simulations applied to industrial processes (oral communication)
P. Gamallo

Efficient transport and magnetoresistance effect in single-molecule devices (oral communication)
E. Ruiz

2nd International Caparica Christmas Congress on Translational Chemistry
Lisbon (Portugal), 4-7 December 2017

Aromaticity of closo boron hydride clusters is driven by Hückel's rule (oral communication)
J. Poater, M. Solà, C. Viñas, F. Teixidor

Chemistry as Innovating Science (CHAINS 2017)
Veldhoven (Netherlands), 5-7 December 2017

Magnetic fingerprint of self-assembling DTA-based molecular magnets (oral communication)
T. Francese

UK Catalysis Hub Winter Conference 2017
Oxfordshire (United Kingdom), 14-15 December 2017

Transition metal carbides based catalysts for clean energy (invited talk)
F. Illas

RESEARCH STAYS IN RECOGNIZED CENTERS

Albertí, M.	**Univeristà di Perugia, Perugia (Itàlia)** Research stay. Dipartimento di Chimica, Biologia e Biotecnologie. February-July 2017
Alemany, P.	**Departamento de Química, Universidad Católica del Norte**, **Antofagasta (Chile)** Invited visiting researcher UB invited by J. Llanos. October 2017
Díez-Pérez, I.	**Department of Chemistry, Kings College London**, **London (United Kingdom)** Invited visiting researcher UB. October-December 2017
López, M.	**Laboratoire d'Electrochimie Moléculaire, UMR CNRS, Université Paris 7, Paris, (France)** PhD research stay. March-May 2017
Mondelo, M.	**Fakultät für Chemie, Universität Bielefeld, Bielefeld (Germany)** PhD research stay with Prof. U. Manthe. February-March 2017
Neyman, K. M.	**Uppsala University, Uppsala (Sweden)** Invited visiting researcher. January-February 2017
Neyman, K. M.	**Chalmers University of Technology, Gotemburg (Sweden)** Invited visiting researcher. May-June 2017
Posada, S.	**Cardiff University, Cardiff (United Kingdom)** PhD research stay. May-July 2017
Prats, H.	**Technische Universität München, Munich (Germany)** PhD research stay with Karsten Reuter. September-December 2017
Ribas, J.	**University of Wroclaw, Wroclaw (Poland)** Invited visiting researcher UB invited by Przemyslaw Dopieralski. July 2017
Ribas, J.	**Center for Computational Science and E-Systems, Japan Atomic Energy Agency, Chiba (Japan)** Invited visiting researcher UB invited by Motoyuki Shiga. October-November 2017

PARTICIPATION IN COMPETITIVE FUNDED RESEARCH PROJECTS

Force Fields in Electrostatic Catalysis
Ismael Díez-Pérez
Universitat de Barcelona
ERC, 2017-2022
European Research Council

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 Bioquímica Integrativa
Marta Cascante Serratosa, Universitat de Barcelona
2014SGR1017, 2014-2017
Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR)

Simulació molecular aplicada (MOLSIMAP)
Fèlix Lluís Llovell Ferret, IQS, Universitat Ramon Llull
2014SGR1582, 2014-2017
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)

Premi a l'Excel.lència Investigadora
Eliseo Ruiz, Universitat de Barcelona
2017
Real Sociedad Española de Química

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)

Reactivity of lattice oxygen in nanostructured CeO_2 doped by Pt and Pd
Konstantin Neyman, Universitat de Barcelona
QCM-2017-2-0024, 2017-2018
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)

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 (MINECO)

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, 2016-2018
Ministerio de Economia y Competitividad (MINECO), Unió Europea

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 (prorrogado)
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, 2015-2018
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)

Fenòmens de no-equilibri en matèria tova: de fluids complexes a teixits cel·lulars
Francesc Sagués Mestre, Universitat de Barcelona
FIS2016-78507-C2-1-P, 2017-2019
Ministerio de Economia y Competitividad (MINECO)

Instituto Nacional de Bioinformática
Marta Cascante Serratosa, Universitat de Barcelona
Ayudas para proyectos de investigación del área de Ciencias de la Salud (FIS), 2018-2020
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,** 2014-2017
Contracto de arrendamientos y servicios de I+D con REPSOL, S.A.

Value added products for cosmetic from soybean by-product. Project DIOR-Barcelona
Francesc Mas Pujadas, Universitat de Barcelona
Contracte amb empresa multinacional BUNGE IBÉRICA SAU, 2017-2018

Estudi de laboratori i planta pilot per la recuperació d'amoni dels purins
Francesc Mas Pujadas, Universitat de Barcelona
Contracte amb empresa multinacional INDUKERN (divisió veterinària), 2017-2019

EXCIPHOCAT: - Tailoring the TiO_2 excited states by nanostructuring and hydroxylation: A step forward understanding photocatalytic water splitting
Francesc Illas Riera
Universitat de Barcelona
PRACE - 2016163940, 2017-2018
Partnership for Advanced Computing in Europe (PRACE)

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)

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

Patient Miner
José Roca Torrent
H2020-EIT. European Institute of Innovation and Technology, 2016-2017
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

Theoretical Chemistry and Computational Modelling
J. J. Novoa, Universidad Autonoma de Madrid
TCCM-642294, 2015-2018
Unió Europea (Marie Skłodowska-Curie Innovative Training Networks)

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)

Addressing CI&TD problems, decreasing drop-out and improving Student outcomes, using active learning methodologies
Joao Luis Monney de Sá Paiva (coordinador Universitat de Viseu), Xavier Giménez (coordinador UB)
Projecte d'Innovació Docent (Universitat de Viseu, Portugal)

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

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

Materiales nanoestructurados en catálisis: Análisis experimental de hallazgos obtenidos mediante modelización computacional
Konstantin Neyman, Universitat of Barcelona
Universitat de Barcelona
PRX17/00348, 2018
Ministerio de Educación, Cultura y Deporte (MECD)

Institut de Química Teòrica i Computacional