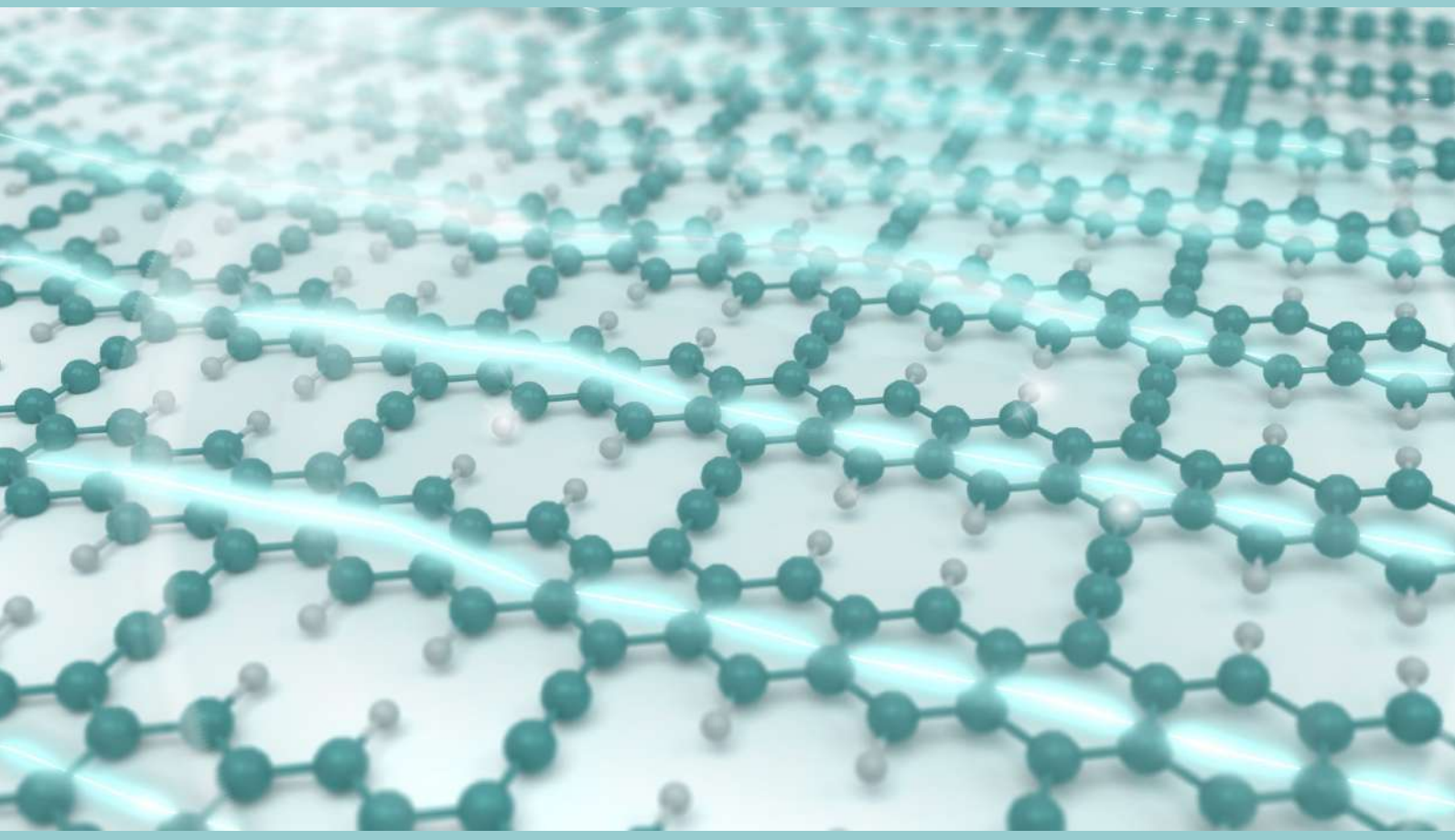
Institut de Química Teòrica i Computacional

EXCELENCIA MARÍA DE MAEZTU

UNIVERSITAT DE BARCELONA

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



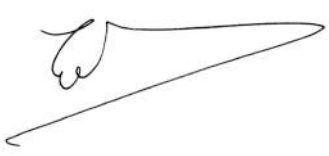
Grazynes: Carbon-Based Two-Dimensional Composites with Anisotropic Properties
The Journal of Physical Chemistry C

Activity Report 2019

The creation of the Institute of Theoretical and Computational Chemistry of the *Universitat de Barcelona* (IQTCUB) was approved by the University's Government Council in ordinary session in November 21st, 2007. From April 2018 I have the honour to serve as Director and I want to take the opportunity of being at the forefront of the IQTCUB's annual memory for acknowledging explicitly to Dr. Jordi Poater for his participation in the previous IQTCUB's direction team and also to Dr. Carles Curutchet for incorporating to the direction team. Additionally, form the point of view of external recognition the María de Maeztu awarding has allowed to incorporate new grant holders and postdocs to the Institute that give us an increase in the quality and quantity of our research. Another important point has been the incorporation of senior researchers through programs like Beatriu de Pinós, Juan de la Cierva, Ramón y Cajal and ICREA.

The common objective of the research projects developed in the Institute is the use of quantum chemistry methods, although recently with the inclusion of experimental groups from our departments new collaborations have started beyond Computational Chemistry fomenting and increasing the multidisciplinary character of our research. Traditionally, the IQTCUS's research is different to that everyone expects for a traditional chemist, since the instrumentation used for our researchers is not found in a traditional laboratory but in a computational "laboratory" that usually is the entrance point to our resources or into supercomputing centres with computational capacity even higher.

The main objective of Theoretical and Computational Chemistry is to achieve the detailed understanding of chemical and physical processes for helping to interpret the experimental results and make predictions that lead to new experiments. According to that, this discipline can provide with new concepts that allow progressing in different aspects like the rational design of new materials with specific physical properties and in their application in electronics and magnetic devices; in the discovery of new medicines and in the understanding of the biochemical processes behind; in new reactions that improve the chemical processes for making them more effective and more environmentally-friendly; and in proposing new sustainable energy sources to overcome the challenges our society faces today. Moreover, we have to integrate in our research new tools like the automatic learning (artificial intelligence), virtual reality and new computational resources ("exascale" and quantum computation).



Eliseo Ruiz
Director of IQTCUB

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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

The IQTCUB direction team during 2019 has been,

Prof. Eliseo Ruiz Sabin	*Director*
Prof. Carles Curutchet Barat	*Secretary (Sept-Dec)*
Prof. Jordi Poater Teixidor	*Secretary (Jan-Sept)*
Prof. Francesc Illas Riera	*Board member*

I.2 IQTCUB RESEARCH LINES

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

1. **Clean and sustainable energy**

What are the mechanisms of crucial chemical processes in energy conversion? Computational chemistry modelling can help in the design of new catalytic materials that can be crucial for electricity production in fuel-cell systems, as well as the catalysts involved in the activation of CO_2 and chemical or electrochemical conversion into useful molecules such as methane, ethylene or ethanol. Furthermore, theoretical approaches could also provide valuable insights into the mechanisms of the oil-water-rock interactions involved in the enhancement of oil recovery.

2. **Nanomaterials and nanoelectronics**

Which chemical compounds exhibit the best magnetic or electron transport properties? The analysis through electronic structure methods provides an accurate understanding of the physical basis of these properties. The most promising molecular materials can include organic radicals, coordination compounds and 2D or 3D materials, that are technologically interesting due to their energy transfer, electronic and magnetic properties, in the search of multifunctional and switchable materials. Computational studies are extremely helpful to implement experiments with appealing targets to be synthesized.

3. **Biomedicine and Soft Matter**

What are the key molecular mechanisms in biological systems? Simulations involving thousands of atoms can be applied to model biomaterials and molecular mechanisms in biologically relevant molecules. Theoretical approach and the implementation of quantum chemistry and mechanical chemistry is useful to investigate the structure and reactivity of proteins and enzymes, to design new drugs, to describe processes in cellular membranes, enzymatic reactions in crowded media and soft nanoparticles in solution.

I.3 IQTCUB MEMBERS

IQTCUB involves a total of 101 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	Gender	Depart./Unit (Section)
Full Professors			
Aguilar Navarro	Antonio	M	Materials Science & Physical Chemistry
Alemany i Cahner	Pere	M	Materials Science & Physical Chemistry
Alvarez Reverter	Santiago	M	Inorganic Chemistry & Organic Chemistry
Aullón López	Gabriel	M	Inorganic Chemistry & Organic Chemistry
Bofill Villà	Josep Maria	M	Inorganic Chemistry & Organic Chemistry
González Pérez	Miguel	M	Materials Science & Physical Chemistry
Illas Riera	Francesc	M	Materials Science & Physical Chemistry
Luque Garriga	Francisco J.	M	Nutrition, Food Sciences & Gastronomy
Mas Pujadas	Francesc	M	Materials Science & Physical Chemistry
Novoa Vide	Juan José	M	Materials Science & Physical Chemistry
Rubio Martínez	Jaime	M	Materials Science & Physical Chemistry
Ruiz Sabin	Eliseo	M	Inorganic Chemistry & Organic Chemistry
Sayós Ortega	Ramón	M	Materials Science & Physical Chemistry
Associate Professors			
Costa Sala	Ramón	M	Inorganic Chemistry & Organic Chemistry
D. P. Ribeiro Moreira	Iberio	M	Materials Science & Physical Chemistry
Giménez Font	Xavier	M	Materials Science & Physical Chemistry
Huarte Larrañaga	Fermín	M	Materials Science & Physical Chemistry
Lucas Alcorta	Josep Maria	M	Materials Science & Physical Chemistry
Llunell Marí	Miquel	M	Materials Science & Physical Chemistry
Mota Valeri	Fernando	M	Materials Science & Physical Chemistry
Paniagua Valle	Juan Carlos	M	Materials Science & Physical Chemistry
Solé Sabaté	Albert	M	Materials Science & Physical Chemistry
Sousa Romero	Carme	F	Materials Science & Physical Chemistry
Vilaseca Font	Eudald	M	Materials Science & Physical Chemistry

Other Categories (Professors Agregats)

Bonet Ruiz	Jordi	M	Chem. Engineering & Analytical Chem.
Curutchet Barat	Carles E.	M	Pharm. & Pharm. Tech. & Phys. Chem.
Deumal Solé	Mercè	F	Materials Science & Physical Chemistry
Gamallo Belmonte	Pablo	M	Materials Science & Physical Chemistry
Madurga Díez	Sergio	M	Materials Science & Physical Chemistry
Ribas Ariño	Jordi	M	Materials Science & Physical Chemistry
Reigada Sanz	Ramón	M	Materials Science & Physical Chemistry
Viñes Solana	Francesc	M	Materials Science & Physical Chemistry

ICREA Research Professors

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

Other Categories (Professors Lectors)

Bidon-Chanal Badia	Axel	M	Nutrition, Food Sciences & Gastronomy
Cirera Fernández	Jordi	M	Inorganic Chemistry & Organic Chemistry
Jover Modrego	Jesús	M	Inorganic Chemistry & Organic Chemistry
Plesu Popescu	Alexandra Elena	F	Chem. Engineering & Analytical Chem.

Other Categories (Professors Associats)

Corbella Morató	Marina	F	Pharm. & Pharm. Tech. & Phys. Chem.
Cremades Martí	Eduard	M	Inorganic Chemistry & Organic Chemistry
Figueras Valls	Marc	M	Materials Science & Physical Chemistry
Ginex	Tiziana	F	Nutrition, Food Sciences & Gastronomy
Jurado Mañas	Anabel	F	Materials Science & Physical Chemistry
López Marne	Estefanía	F	Materials Science & Physical Chemistry
Piqué Caufapé	Oriol	M	Materials Science & Physical Chemistry
Tercero Mohedano	Javier	M	Inorganic Chemistry & Organic Chemistry
Valero Montero	Rosendo	M	Materials Science & Physical Chemistry
Viayna	Antonio	M	Nutrition, Food Sciences & Gastronomy

Postdoctoral contracts

Beatriu de Pinós-Juan de la Cierva

Gómez Coca	Silvia	F	Inorganic Chemistry & Organic Chemistry
Morales García	Ángel	M	Materials Science & Physical Chemistry

Ramón y Cajal

Calle Vallejo	Federico	M	Materials Science & Physical Chemistry
Echeverría López	Jorge	M	Inorganic Chemistry & Organic Chemistry

Contracte Projecte de Recerca

De Souza Pinheiro	Silvana	F	Pharm. & Pharm. Tech. & Phys. Chem.
Escartín Esteban	José María	M	Inorganic Chemistry & Organic Chemistry
Prats García	Hèctor	M	Materials Science & Physical Chemistry
Valero Montero	Rosendo	M	Materials Science & Physical Chemistry

Other

Abrahao B. de Morais	Mariana	F	Inorganic Chemistry & Organic Chemistry
Albareda Piquer	Guillem	M	Inorganic Chemistry & Organic Chemistry
Vilà Casanova	Arnau	M	Materials Science & Physical Chemistry

Ph.D. Students

Beca Programa María de Maeztu

Colomer Llombart	Eduard	M	Materials Science & Physical Chemistry
Gonzalo Palao	Daniel	M	Pharm. & Pharm. Tech. & Phys. Chem.
Lleopart Motis	Genis	M	Materials Science & Physical Chemistry
Morales Salvador	Raúl	M	Materials Science & Physical Chemistry
Privat Contreras	Cristian	M	Materials Science & Physical Chemistry
Vidal Ramon	Daniel	M	Química Inorgànica i Química Orgànica
Vílchez	David	M	Nutrition, Food Sciences & Gastronomy

FI Grant (Catalan Government Program)

Aledavood	Elnaz	F	Nutrition, Food Sciences & Gastronomy
Balcells Nadal	Cristina	F	Materials Science & Physical Chemistry
Blanco Andrés	Pablo Miguel	M	Materials Science & Physical Chemistry
Lozano Reis	Pablo	M	Materials Science & Physical Chemistry
Macià Escatllar	Antoni	M	Materials Science & Physical Chemistry
Nin Hill	Alba	F	Inorganic Chemistry & Organic Chemistry

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

Almacellas Salillas	David	M	Inorganic Chemistry & Organic Chemistry
Bernuz Fitó	Efrem	M	Materials Science & Physical Chemistry
Coines López-Nieto	Joan	M	Inorganic Chemistry & Organic Chemistry
Esquivias Baut. Lisb.	Oriol	M	Inorganic Chemistry & Organic Chemistry
Martín Rodríguez	Alejandro	M	Inorganic Chemistry & Organic Chemistry
Piñero Vargas	Juan José	M	Materials Science & Physical Chemistry
Santiago Piera	Raúl	M	Materials Science & Physical Chemistry

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

Amoza Dávila	Martín	M	Inorganic Chemistry & Organic Chemistry
Vilaplana Saiz	Marta	F	Materials Science & Physical Chemistry

ITN UE Grant

Francese	Tommaso	M	Materials Science & Physical Chemistry
Mnevets	Daniil	M	Inorganic Chemistry & Organic Chemistry

UB / ADR Grant (University of Barcelona own programme) / APIF

Blancafort Jorquera	Miquel	M	Materials Science & Physical Chemistry
López Berbel	Martí	M	Materials Science & Physical Chemistry
Roncero Barrero	Cristina	F	Materials Science & Physical Chemistry
Svobodova	Adela	F	Materials Science & Physical Chemistry
Velásquez Benites	Juan Diego	M	Inorganic Chemistry & Organic Chemistry

Beca CONICYT

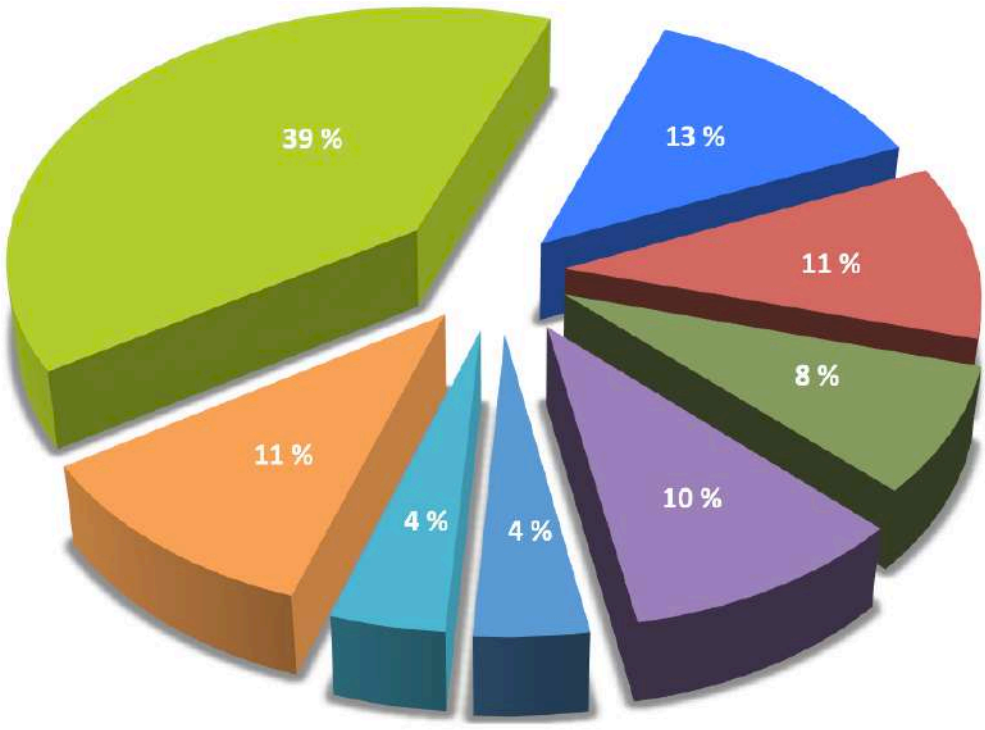
Zamora	William J.	M	Nutrition, Food Sciences & Gastronomy

Beca Doctorat Industrial

Espel Grekopoulos	Joan	M	Pharm. & Pharm. Tech. & Phys. Chem.
Vázquez López	Javier	M	Nutrition, Food Sciences & Gastronomy

Other

Alonso Benito	Gerard	M	Materials Science & Physical Chemistry
Barazorda-Ccahuana	Haruna	F	Materials Science & Physical Chemistry
Cánovas Montes	Manuel Anto.	M	Materials Science & Physical Chemistry
Kamalinahad	Saedeh	F	Materials Science & Physical Chemistry
Ozaydin	Gül Beste	F	Pharm. & Pharm. Tech. & Phys. Chem.
Saranjam	Leila	F	Materials Science & Physical Chemistry
Vega Domínguez	Lorena	F	Materials Science & Physical Chemistry
Vila Julià	Guillem	M	Materials Science & 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 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 175.000 €*)

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 75.000 €*)

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

2 Nodes AZServer 4G3S
CPU: 2 x 2,2 GHz Dual Xeon E5-2600v4 (10 cores)
RAM: 128 GB
HD: 2 x 2 TB hard disk
Network: 4 gigabit network card + 1 IPMI card (OOB)
GPU: 4 NVIDIA GEFORCE GTX 1070Ti

SERVERS

Glusterfs disk server (*invested value 54.000 €*)

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)

Machine type Supermicro
Operating system Centos 7.6

Services Storage service cluster with 64TB of space for applications directories and user's work area exported by NFS
Structure 1 node
Notes Storage service redundant power supply

Specifications:

1 Node Supermicro 2U
CPU: 2 x 2,20 GHz Xeon 4210
RAM: 64 GB
HD: 8 x 8 TB (raid 5)
Network: 4 gigabit network card
Network: 2 10GB network card

Machine type DELL
Operating system Centos 7.6
Services Storage service cluster with 100TB of space for applications directories and user's work area exported by GlusterFS
Structure 1 node
Notes Storage service redundant power supply
Specifications:

1 PowerEdge R740XD
CPU: 2 x 2,10 GHz Xeon 4110
RAM: 64 GB
HD: 10 x 10 TB (raid 5)
Network: 4 gigabit network card
Network: 2 10GB network card

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 28.300 €*)

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)

Machine type	1 node
Operating system	Centos 7.3
Services	Pre-production and testing proposals
Structure	1 node

Specifications:

1 DELL PowerEdge R640
CPU: 2 x 2 GHz Xeon Gold 6138
RAM: 128 GB
HD: 2 x 2 TB (raid 1)
Network: 2 gigabit network card + iDrac

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).
13. 1 MSI LAPTOP with Oculus RIFT S -Virtual Reality Study-.

The approximated invested cost of this equipment is *53.000 €.*

SUMMARY

Cores.....4,062 c

Memory ..... 38,886 GB RAM

Calculation disk capacity.....266 TB

Data user disk capacity.....132 TB

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

*2.100.000 €**

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

II. IQTCUB ACTIVITIES

II.1 GENERAL ACTIVITIES

Next, a description of activities and actions promoted by IQTCUB through 2019 is provided.

a. ***Promotion and encouragement of research.*** This year the IQTCUB has finally offered one 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 Silvia Sodric for starting Master studies under the supervision of Dr. Jordi Poater.

Total cost: 2.680 €

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

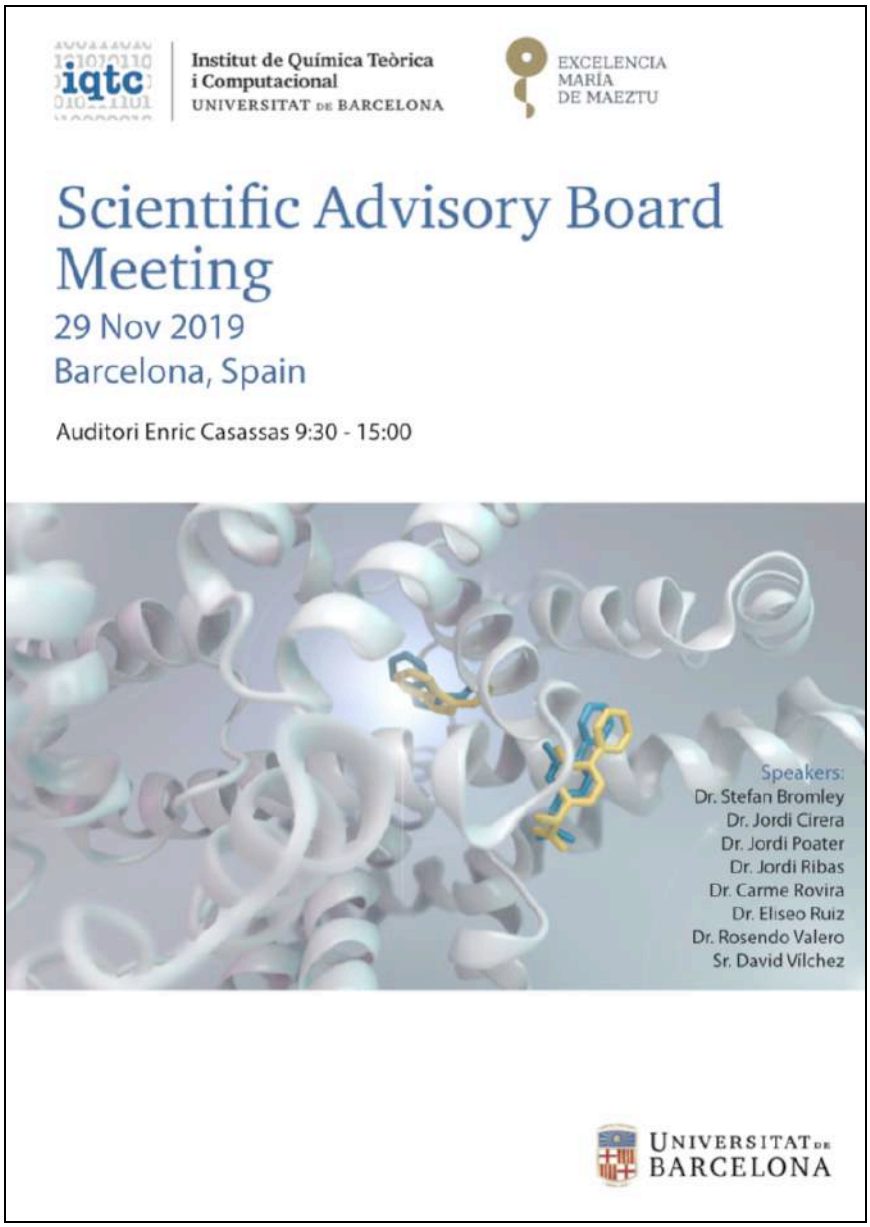
b. ***10th IQTCUB workshop.*** This one-day workshop aimed at the dissemination of the research done at the IQTCUB took place on May 31st, 2019 at it was organized by Dr. Jordi Cirera. The IQTCUB members and internationally acknowledged speakers present the most recent work. This year we highlight the participation of Prof. Dr. Martin Kaupp from the Technische Universität Berlin with the invited lecture entitled *New Quantum Methods and New Applications: NMR/EPR Parameters, Local Hybrid Functionals, and more*, and Prof. Dr. John E. McGrady from the University of Oxford with the invited lecture entitled *Pushing molecules around: a theoretical perspective on the chemical bond, and how to modify it*. The other invited speakers were Dr. Axel Bidon-Chanal (*Computational biology and gastronomy research in the food and nutrition Torribera campus*), Joan Coines (*Mechanistic insights into substrate- assisted glycoside hydrolases*) and Antoni Macià (*A computational view on astronomical silicate nanoclusters*) all three from University of Barcelona and IQTCUB. Moreover, 17 poster contributions have been presented during the meeting (https://www.iqtc.ub.edu/news/posters-at-the-iqtcub-symposium-2019/). The IQTCUB assigned a budget to cover the traveling and lodging expenses of the invited professors as well as the catering service offered to all assistants.

Total cost: 1.491 € + 2.000 € economic assignment of Faculty of Chemistry

Panel of the *10th IQTCUB workshop*.

c. ***IQTC Scientific Advisory Board Meeting.*** On November 29th 2019 it was held the first IQTCUB scientific advisory meeting with the participation of Profs. Agustí Lledós (Universitat Autònoma de Barcelona), John McGrady (University of Oxford), Sofía Calero (Universidad Pablo de Olavide), Federico Gago (Universidad de Alcalà), Carmen Domene (University of Bath) i Roser Valentí (Goethe-Universität Frankfurt).

Total cost: 3.650 €



Panel of the *meeting*.

df. ***Scientific Dissemination Activities.*** Prof. Xavier Giménez Font has been involved in the following scientific and teaching dissemination activities during 2019:

1. "UB s'Apropa 19". INS Domènec Perramon, Arenys de Munt, 9/Jan/2019.
2. "UB s'Apropa 19". INS Manuel Blancafort, La Garriga, 11/Jan/2019.
3. "UB s'Apropa 19". INS Miramar, Viladecans, 11/Jan/2019.
4. "Les Microones i les Ones de Ràdio. Què són i com ens afecten?", Toc–Toc UB Science Dissemination Program, INS Miquel Bosch i Jover, Artés. 15/Jan/2019.
5. "Apropa't a la UB!". Visit of INS JM Quadrado, La Ciutadella (Menorca). Universitat de Barcelona, 16/Jan/2019.
6. "UB s'Apropa 19". INS Vil·la Romana, La Garriga, 16/Jan/2019.
7. "UB s'Apropa 19". INS Gallecs, Mollet del Vallès, 18/Jan/2019.
8. "UB s'Apropa 19". EDUCEM II, Granollers, 23/Jan/2019.
9. "UB s'Apropa 19". INS Sentmenat, Sentmenat, 23/Jan/2019.
10. "UB s'Apropa 19". INS La Roca, La Roca del Vallès, 24/Jan/2019.
11. "UB s'Apropa 19". INS Escola del Treball, Granollers, 29/Jan/2019.
12. "UB s'Apropa 19". Escola Sant Gabriel, Sant Adrià del Besòs, 29/Jan/2019.
13. "UB s'Apropa 19". INS Lluís Domènech i Montaner, Canet de Mar, 30/Jan/2019.
14. "UB s'Apropa 19". INS Pau Vila, Sabadell, 30/Jan/2019.
15. "UB s'Apropa 19". INS Lauro, Les Franqueses del Vallès, 31/Jan/2019.
16. "UB s'Apropa 19". INS Vilamajor, Sant Pere de Vilamajor, 1/Feb/2019.
17. "UB s'Apropa 19". INS Gallecs, Mollet del Vallès, 1/Feb/2019.
18. "UB s'Apropa 19". INS Vall del Tenes, Santa Eulàlia de Ronçana, 4/Feb/2019.
19. "UB s'Apropa 19". INS Alba del Vallès, Group A, Sant Fost de Campsentelles, 5/Feb/2019.
20. "UB s'Apropa 19". INS Alba del Vallès, Group B, Sant Fost de Campsentelles, 5/Feb/2019.
21. "UB s'Apropa 19". Escola Jesuites Sant Gervasi – Infant Jesús, Barcelona, 6/Feb/2019.
22. "UB s'Apropa 19". INS Miramar, Viladecans, 8/Feb/2019.
23. "UB s'Apropa 19". INS Torre de Malla, Parets del Vallès, 20/Feb/2019.

24. “UB s’Apropa 19”. INS Polinyà, Polinyà, 22/Feb/2019.
25. “UB s’Apropa 19”. INS Lauro, Les Franqueses del Vallès, 28/Feb/2019.
26. “UB s’Apropa 19”. INS Lliçà, Social & Human Sci. students, Lliçà d’Amunt, 1/Mar/2019.
27. “UB s’Apropa 19”. INS Lliçà, Technology & Science students, Lliçà d’Amunt, 1/Mar/2019.
28. “UB s’Apropa 19”. Escola Pia, Caldes de Montbui, 13/Mar/2019.
29. “La màgia de l’aigua”, Toc–Toc UB Science Dissemination Program, Centre Cívic El Sortidor, Barcelona. 13/Mar/2019.
30. “La màgia de l’aigua”, VIII Diada de la Ciència, 2019, Escola Pia, Caldes de Montbui. 14/Mar/2019.
31. “Les Microones i les Ones de Ràdio. Què són i com ens afecten?”, Toc–Toc UB Science Dissemination Program, Escola Sant Gabriel, Sant Adrià del Besòs, 18/Mar/2019.
32. “UB s’Apropa 19”. INS Celestí Bellera, Granollers, 19/Mar/2019.
33. “UB s’Apropa 19”. INS Mollet, Mollet del Vallès, 20/Mar/2019.
34. “UB s’Apropa 19”. INS Torres i Bages, Hospitalet de Llobregat, 20/Mar/2019.
35. “Apropa’t a la UB!”. Visit of Escola Lleó XIII. Universitat de Barcelona, 22/Mar/2019.
36. “Com es creen els elements químics? Quins formen el nostre cos?”, Visions de Ciència Series, Biblioteca Sagrada Família, Barcelona. 25/Mar/2019.
37. “La Màgia de l’Aigua”. Toc–Toc UB Science Dissemination Program, INS Salvador Dalí, El Prat de Llobregat, 26/Mar/2019.
38. “UB s’Apropa 19”. INS Torres i Bages, Hospitalet de Llobregat, 27/Mar/2019.
39. “La Màgia de l’Aigua”. Pessics de Ciència Program, Centre Cultural Sant Josep, Hospitalet de Llobregat, 27/Mar/2019.
40. “UB s’Apropa 19”. INS Vinyet, Sitges, 28/Mar/2019.
41. “UB s’Apropa 19”. INS Manolo Hugué, Caldes de Montbui, 12/Apr/2019.
42. “UB s’Apropa 19”. INS Eugeni Xammar, L’Ametlla del Vallès, 26/Apr/2019.
43. “UB s’Apropa 19”. Escola Lleó XIII, Barcelona, 3/May/2019.
44. “Mechanochemistry – Macroscopic versus Microscopic Mechanics and Dynamics”. Key–note talk at “Symposium on Movement Technologies”, University of Applied Sciences and Arts – Dortmund, Dortmund, Germany, 23/May/2019.

45. “Les Microones i les Ones de Ràdio. Què són i com ens afecten?”, Toc–Toc UB Science Dissemination Program, Biblioteca Sagrada Família, Barcelona. 5/Jun/2019.
46. “La Màgia de l’Aigua”. Toc–Toc UB Science Dissemination Program, Institut Castellbisbal, Castellbisbal, 1st Group, 4/Oct/2019.
47. “La Màgia de l’Aigua”. Toc–Toc UB Science Dissemination Program, Institut Castellbisbal, Castellbisbal, 2nd Group, 4/Oct/2019.
48. “La Màgia de l’Aigua”. Toc–Toc UB Science Dissemination Program, Institut Castellbisbal, Castellbisbal, 3rd Group, 4/Oct/2019.
49. “Llibres de Divulgació Científica”, Màster de Comunicació Científica, Univ. Barcelona, 28/Oct/2019.
50. “L’origen dels elements químics”, 8es Jornades Ensenyament de la Química a Catalunya, Facultat de Química, Universitat de Barcelona, Barcelona, 6/Nov/2019.
51. “L’origen dels elements químics”, La Setmana de la Ciència 2019, CRP Garraf, Universitat Politècnica de Catalunya, Vilanova i la Geltrú, 11/Nov/2019.
52. “La màgia de l’aigua”, La Setmana de la Ciència 2019, La Salle Bonanova, Barcelona. 12/Nov/2019.
53. “La màgia de l’aigua”, La Setmana de la Ciència 2019 i Toc–Toc UB Science Dissemination Program, Institut Jaume Salvador, Sant Joan Despí. 20/Nov/2019.
54. “L’Aire que Respirem”, Toc–Toc UB Science Dissemination Program, Escola Immaculada Concepció, Barcelona. 21/Nov/2019.
55. “L’Aire que Respirem”, Toc–Toc UB Science Dissemination Program, Institut Montserrat Roig, Barcelona. 27/Nov/2019.
56. “La Màgia de l’Aigua”. Toc–Toc UB Science Dissemination Program, Escola Patronat Domènech, Barcelona, 20/Dec/2019.

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

1. "A la caza del CO_2", interviewed by Andrea Nogueira.
   El Pais Journal, January 6th, 2019.
   https://elpais.com/cultura/2019/01/04/actualidad/1546601992_837620.html

2. "La Màgia de l'Aigua", Conference within the series "Pessics de Ciència", Centre Cultural Sant Josep.
   L'Hospitalet de Llobregat, March 27th, 2019.
   https://www.youtube.com/watch?v=3oRJf6LEvug&feature=youtu.be

3. "SABER: Let's make high students performance possible, even in STEM courses", METID & Faculty seminar.
   Istituto Politecnico di Milano, May 16th, 2019.
   https://www.youtube.com/watch?v=gIjsJ1uYPm0&feature=youtu.be

4. "El mejor truco para enfriar bebidas a toda velocidad sin congelador", nterviewed by Anna Macià for "Comer" section of La Vanguardia Journal, July 3rd, 2019
   https://www.lavanguardia.com/comer/tendencias/20190627/463134511552/enfriar-bebidas-ola-de-calor-refrescos-velocidad-rapido.html?fbclid=IwAR26NWDDnwllDxdyTpgPdyx7IabIYNCdTaFJqy5CgKBl5u87TCJwdcweh0I

5. "Fem possible un ensenyament universtari de qualitat", interviewed by Antoni Portell, Director of CIFE, Centre d'Innovació i Formació en Educació, Universitat de Vic, July 16th, 2019
   https://mon.uvic.cat/cife/xavier-gimenez-ensenyar-de-forma-entenedora-eficient-i-engrescadora-es-mes-possible-que-mai-i-es-a-labast-de-tots/

6. "N'hi ha prou amb prohibir els cotxes vells? Deu coses que pot fer Barcelona contra la crisi climàtica", interviewed by Andreu Merino, Nacio Digital journal. October 3rd, 2019
   https://www.naciodigital.cat/noticia/188363/prou/amb/prohibir/cotxes/vells/deu/coses/pot/fer/barcelona/contra/crisi/climatica

7. "Què són les bateries d'ió–liti, el motiu del Premi Nobel de Química d'enguany", interviewed by Sandra Mestres, betevé notícies vespre program, Betevé Televisió, Barcelona, October 11th, 2019
   https://beteve.cat/btv-noticies-vespre/btv-noticies-vespre-1388/

8. "Els filtres de partícules als motors diésel", interviewed by Xavier Muixí, Betevé Notícies Vespre program, Betevé Televisió, Barcelona, November 27th, 2019
   https://beteve.cat/btv-noticies-vespre/btv-noticies-vespre-1427/

Other dissemination activities carried out for IQTC members during 2019 are the following:

1. *"Fem Química al Laboratori"*
   Antonio Aguilar, Carme Sousa i Pablo Gamallo, January-February 2019.

2. *"V Festa de la Ciència de la UB"*
   Hèctor Prats, Pablo Gamallo, University of Barcelona, 17 May 2019.
   http://www.ub.edu/laubdivulga/festacienciaub/festacienciaV/index.html

II.2 IQTCUB SEMINARS AND CONFERENCES

During 2019 Dr. Jordi Poater has organized the following IQCT's seminars and conferences:

1. **Dr. Maytal Caspary** (Israel Institute of Technology), Haifa, Israel.
   Recent advances in modeling Fe_2O_3 for water splitting catalysis
   23 January 2019.

2. **Dr. Umberto Terranova** (University of Cardiff) Cardiff, United Kingdom.
   Iron sulphide minerals: phase stability and oxidation behavior
   8 February 2019.

3. **Dr. Alejandro Rodríguez** (Int. Center of Theoretical Physics), Trieste, Italy.
   The fuzzy border between Molecular Simulations and data science
   5 March 2019.

4. **Dr. Mercedes Alfonso** (IAS-5, INM-9), Jülich, Germany.
   Understanding ligand selectivity in bitter taste receptors using multiscale molecular dynamics simulations
   22 March 2019.

5. **Prof. Aliaksandr Bandarenka** (Technische Universität München), Munich, Germany.
   Why electrolytes control the catalytic activity
   8 April 2019.

6. **Dr. Taehum Lee** (Yonsei University), Seoul, South Korea.
   Characterization of ultrathin oxidic metal layers on another surrogate metal support: A theoretical surface science approach
   9 April 2019.

7. **Dr. Julian Gebhardt** (Max Planck Institute), Hamburg, Germany.
   New Materials from Simulations
   26 April 2019.

8. **Prof. Anela Ivanova** (Sofia University), Sofia, Bulgaria.
   Molecular design of new organic TADF emitters
   3 May 2019.

9. **Prof. Vladimir Guterman** (Southern Federal University), Rostov-on-Don, Russia.
   Pt-Containing Nanostructured Electrocatalysts for Low-Temperature Fuel Cells
   21 May 2019.

10. **Prof. Francisco Zaera** (University of California), Riverside, USA.
    The Route to Better Catalysts: From Surface Science to Nanotechnology
    24 May 2019.

11. **Prof. Diana Cheshmedzhieva** (University of Sofia), Sofia, Bulgaria.
    Application of theoretical computations in studying reaction mechanisms and reactivity of organic compounds
    18 June 2019.

12. **Dr. Isaac Alcón** (Freie Universität Berlin), Berlin, Germany.
    Quantum interference engineering of nanoporous graphene for carbon nanocircuitry
    8 October 2019.

13. **Dr. Sergi Vela** (EPFL), Lausanne, Switzerland and (Université Strasbourg) Strasbourg, France.
    Modern Computational Tools to Investigate Spin Crossover and Azoheteroarene-based molecular switches
    21 October 2019.

14. **Prof. Notker Rösch** (Technische Universität München), Munich, Germany.
    Single Atom Catalysis – a Theoretician's Dream Scenario? Lessons from Working on C-C Coupling over Zeolite-supported Rh(I)
    6 November 2019.

15. **Dr. Aleix Comas-Vives** (Universitat Autònoma de Barcelona), Bellaterra, Spain.
    Ab Initio and Multiscale Modelling of CO_2 Conversion to Methanol and Syngas: Active Sites and Selectivity
    11 December 2019.

II.3 IQTCUB INVITED RESEARCHERS

During 2019, a total of twenty-two researchers have spent some time at the IQTCUB collaborating in different research projects.

1. **Prof. Hristiyan Aleksandrov** (invited researcher).
   University of Sofia, Bulgaria.
   January-february, june-august 2019.

2. **Prof. Iskra Koleva** (invited researcher).
   University of Sofia, Bulgaria.
   January-february, june-july 2019.

3. **Dr. Annika Borg** (invited researcher).
   Graz University of Technology, Austria.
   February 2019.

4. **Dr. David Gobrecht** (HPC Europa researcher)
   Katholieke Universiteit Leuven, Belgium.
   February 2019.

5. **Dr. Juan Aragó** (invited researcher).
   Institut de Ciència Molecular de la Universitat de València, Spain.
   March 2019.

6. **MSc. Laura Granda** (HPC Europa researcher)
   Leiden University, Netherlands.
   April-july 2019.

7. **Dr. Ciro Achille** (invited researcher).
   University of Pàdova, Italy.
   May 2019.

8. **Prof. Anela Ivanova** (invited researcher).
   University of Sofia, Bulgaria.
   May 2019.

9. **Prof. Georgi Vayssilov** (invited researcher).
   University of Sofia, Bulgaria.
   June 2019.

10. **Prof. Rositca Nikolova** (invited researcher).
    University of Sofia, Bulgaria.
    June 2019.

11. **Dr. Miroslava Nedyalkova** (invited researcher).
    University of Sofia, Bulgaria.
    June-july 2019.

12. **Prof. Vasil Simeonov** (invited researcher).
    University of Sofia, Bulgaria.
    July 2019.

13. **Dr. Rita Dias** (invited researcher).
    NTNU, Norway.
    October 2019.
    July 2019.

14. **Dr. Lorenzo Mino** (invited researcher).
    Universitá degli Studi di Torino, Italy.
    July-august 2019.

15. **MSc. Cameron Beevers** (HPC Europa researcher).
    Cardiff University, United Kingdom.
    September-november 2019.

16. **Antonio Pantoja** (invited researcher).
    UNAM, Mexico.
    September 2019 – February 2020.

17. **MSc. Hedda Oschinski** (ERASMUS researcher).
    Leibniz University, Germany.
    September 2019 – march 2020.

18. **Dr. Enrico Bisquoli** (invited researcher).
    University of Pisa, Italy.
    October-december 2019.

19. **Dr. Ludivine Levedel** (invited researcher).
    University of Poitiers, France.
    November 2019.

20. **Prof. Maria Hrmova** (invited researcher).
    University of Adelaide, Australia.
    November 2019.

21. **Dr. Giovanni Di Liberto** (HPC Europa researcher).
    Universitá degli Studi di Milano-Bicocca, Italy.
    November-december 2019.

22. **Dr. Massomeh Keyhanian** (invited researcher).
    University of Mazandaran, Iran.
    December 2019 – july 2020.

III. SCIENTIFIC ACTIVITY OF IQTCUB MEMBERS

III.1 HIGHLIGHTS FROM MOST RELEVANT RESULTS

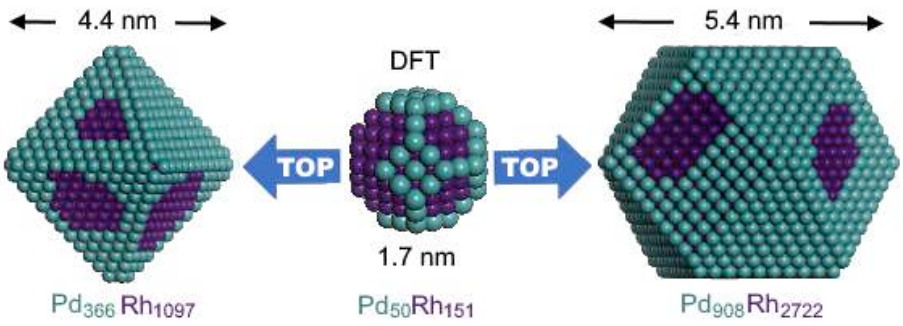
Here some of the most relevant results corresponding to every IQTCUB main research line are presented.

LINE 1. CLEAN AND SUSTAINABLE ENERGY

Using density functional calculations to elucidate atomic ordering of Pd-Rh nanoparticles at sizes relevant for catalytic applications.

L. Vega, H. A. Aleksandrov, K. M. Neyman.

Chinese J. Catal., *40* (2019) 1749.



DFT modelling identifies surface composition of Pd-Rh particles of thousands atoms and paves the way for evaluating surface segregation due to adsorbed reactants.

This study quantifies, with the help of density functional (DFT) calculations and our novel Topological Approach, atomic ordering and surface segregation effects in Pd-Rh particles with compositions 1:3, 1:1 and 3:1 containing up to 201 atoms (ca. 1.7 nm). The obtained data are used to reliably optimise energetically preferred atomic orderings in inaccessible by DFT Pd-Rh particles containing thousands of atoms and exhibiting sizes exceeding 5 nm, which are typical for catalytic metal particles. It is outlined, how segregation effects on the surface arrangement of Pd-Rh nanoalloy catalysts induced by adsorbates can be evaluated in a simple way within the present modelling setup.

Kinetic Monte Carlo simulations unveil synergic effects at work on bifunctional catalysts.

H. Prats, S. Posada-Pérez, J. A. Rodríguez, R. Sayós, F. Illas.

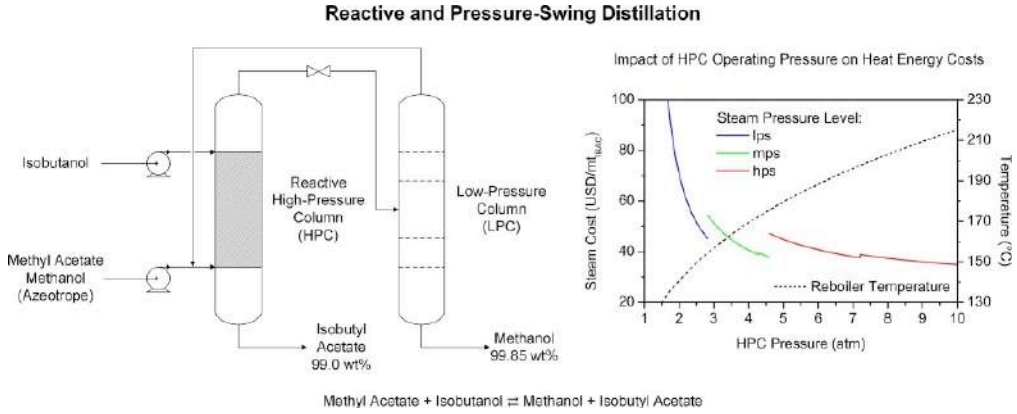
ACS Catal., *9* (2019) 9117-9126.

The interaction between metal particles and the support in heterogeneous catalysis has been the subject of a large number of studies. While strong metal–support interactions can lead to deleterious catalyst deactivation and the underlying mechanism is well understood, in other cases the effect may beneficially enhance the catalytic activity and/or selectivity with no clear picture of the chemistry involved. The kMC simulations provide strong evidence for a cooperative effect between the different regions of the catalyst Au/MoC. Thus, the clean MoC regions are responsible for adsorbing and dissociating water molecules, and the vicinity of the Au adclusters contributes to COOH formation.

Pressure selection for non-reactive and reactive pressure-swing distillation.

A. Risco, V. Plesu, J. A. Heydenreich, J. Bonet, A. E. Bonet-Ruiz, A. Calvet, P. Iancu, J. Llorens.

Chem. Eng. Process – Process Intensification *135* (2019) 9.

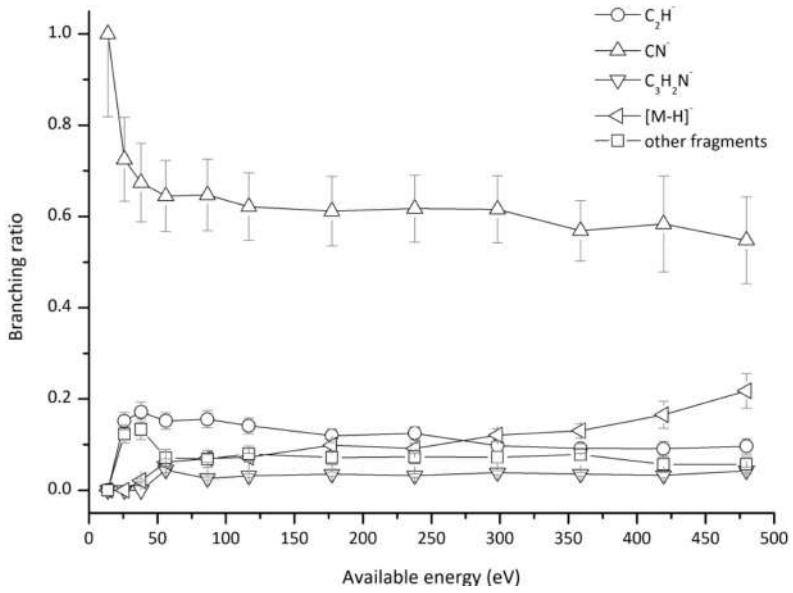


Theoretical study of simulation that shows that when the heating services increase their quality, i.e. low, medium or high pressure steam, their costs increase suddenly. This point must be considered when optimizing the pressure of a pressure swing distillation.

Ion-pair formation in neutral potassium-neutral pyrimidine collisions: electron transfer experiments.

A. M. Mendes; B. Pamplona, S. Kumar; F. Ferreira da Silva, A. Aguilar, G. García, M. C. Bacchus_Montabonel, P. Limao-Vieira.

Front. Chem., *7* (2019) 157.



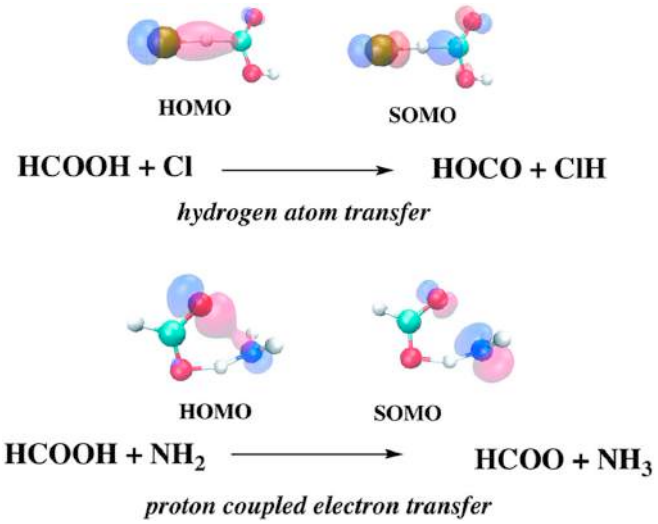
Pyrimidine branching ratios (fragment anion yield/total anion yield) of the main negative ions formed as a function of the collision energy in the center-of-mass frame.

We report on ion-pair formation in hyperthermal (30–800 eV) neutral potassium collisions with neutral pyrimidine molecules. Negative ions formed by electron transfer from the alkali atom to the target molecule were time-of-flight mass analysed and the fragmentation patterns and branching ratios obtained. The most abundant product anions have been assigned to CN^- and C_2H^- and the electron transfer mechanisms are comprehensively discussed. Theoretical calculations were performed for pyrimidine in the presence of a potassium atom and provided a strong basis for the assignment of the lowest unoccupied molecular orbitals accessed in the collision process. In order to further our knowledge about the collision dynamics, potassium cation (K^+) energy loss spectrum has been obtained and within this context, we also discuss the role of the accessible electronic states. A vertical electron affinity of (−5.69 ± 0.20) eV was obtained and may be assigned to a $\pi^*_3(b_1)$ state that leads to CN^- formation.

The gas phase oxidation of HCOOH by Cl and NH_2 radicals. Proton coupled electron transfer versus hydrogen atom transfer.

J. M. Anglada, R. Crehuet, A. Solé.

Mol. Phys., *117* (2019) 1430.



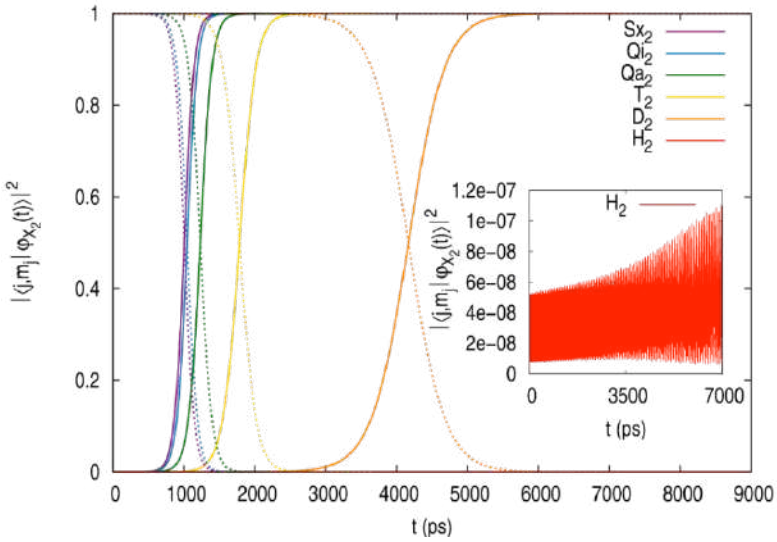
Examples of hat and pcet reaction mechanisms.

The reaction of formic acid (HCOOH) with chlorine atom and amidogen radical (NH_2) have been investigated using high level theoretical methods such BH&HLYP, MP2, QCISD, and CCSD(T) with the 6–311+G(2df,2p), aug-cc-pVTZ, aug-cc-pVQZ and extrapolation to CBS basis sets. The abstraction of the acidic and formyl hydrogen atoms of the acid by the two radicals has been considered, and the different reactions proceed either by a proton coupled electron transfer (pcet) and hydrogen atom transfer (hat) mechanisms. Our calculated rate constant at 298 K for the reaction with Cl is 1.14 x 10^{-13} cm^3 $molecule^{-1}$ s^{-1} in good agreement with the experimental value 1.8±0.12/2.0 x 10^{-13} cm^3 $molecule^{-1}$ s^{-1} and the reaction proceeds exclusively by abstraction of the formyl hydrogen atom, via hat mechanism, producing HOCO+ClH. The calculated rate constant, at 298 K, for the reaction with NH_2 is 1.71 x 10^{-15} cm^3 $molecule^{-1}$ s^{-1}, and the reaction goes through the abstraction of the acidic hydrogen atom, via a pcet mechanism, leading to the formation of HCOO+NH_3.

Rotational energy relaxation quantum dynamics of a diatomic molecule in a superfluid helium nanodroplet and study of the hydrogen isotopes case.

M. Blancafort-Jorquera, A. Vila, M. González.

Phys. Chem. Chem. Phys., *21* (2019) 21007.



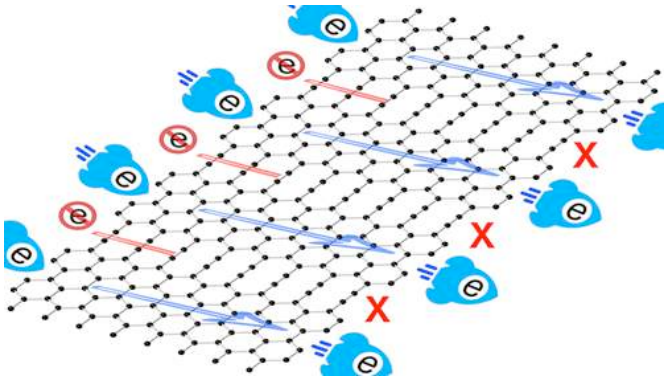
Populations of the (j=0, m_j=0) (solid lines) and (j=2, m_j=0) (dashed lines) rotational states of molecules, as a function of time.

The rotational energy relaxation (RER) of a molecule $X_2(j, m_j)$ in a ^{4}He superfluid nanodroplet [HeND; *T*=0.37 K] was studied using a hybrid quantum dynamics approach proposed by us. This is the first theoretical study about RER in HeNDs and here several isotopes of H_2 were examined. The structure of the HeND does not change during the RER, which takes place according to a cascade mechanism and m_j is conserved. The lifetime of an excited rotational state (≈1.0-7.6 ns) increases when B_e increases, *j* increases, and *N* decreases (above *N*=100 He atoms there is a small influence of *N* on the lifetime). The analysis of the influence of the coupling between the *j* - *j*-2 rotational states and the X_2 angular velocity on the lifetime was helpful to interpret the results. We hope that the present study will encourage more studies on RER in HeND, a basic, interesting and difficult to study phenomenon about which we still know very little.

Grazynes: carbon-based two-dimensional composites with anisotropic properties.

S. Kamalinahad, F. Viñes, P. Gamallo.

J. Phys. Chem. C *123* (2019) 27140.



2D grazynes structures where electronic and elàstic properties are highly dependent on the direction.

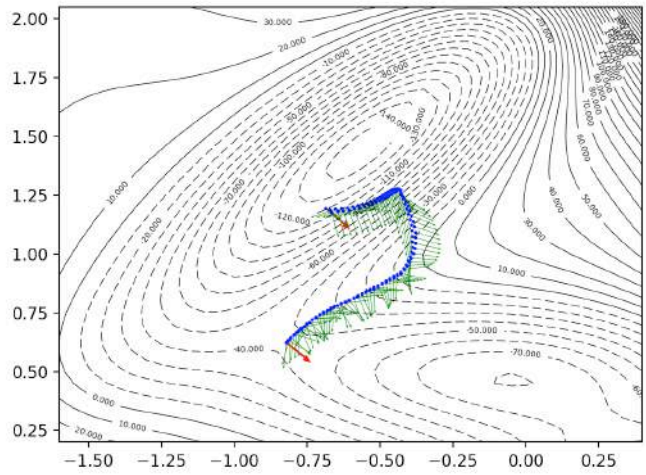
A new family of two-dimensional carbon allotropes is presented, based on graphene stripes linked to each other by acetylenic connections. The large amount of allowed connectivities demands a family name for them: grazynes. The present study reports the energetic, structural, elastic, and electronic physicochemical properties of a set of simple grazynes by means of density-functional-theory-based calculations, suggesting also possible synthetic routes. The main results conclude that these are exotic yet stable materials, stiffer than graphene in the acetylenic direction, highly anisotropic, and with the presence of Dirac points in the reciprocal space along the graphene stripes direction resistant to strain, regardless of its direction. Thus, grazynes infer directionality in electron conductivity and resilience to the material stretching/compression, quite important, for instance, in the nanoelectronics applicability point of view.

LINE 2. NANOMATERIALS AND NANOELECTRONICS

Interplay between the gentlest ascent dynamics method and conjugate directions to locate transition states.

J. M. Bofill, J. Ribas-Ariño, R. Valero, G. Albareda, I. de P. R. Moreira, W. Quapp.

J. Chem. Theory Comp., *15* (2019) 5426.



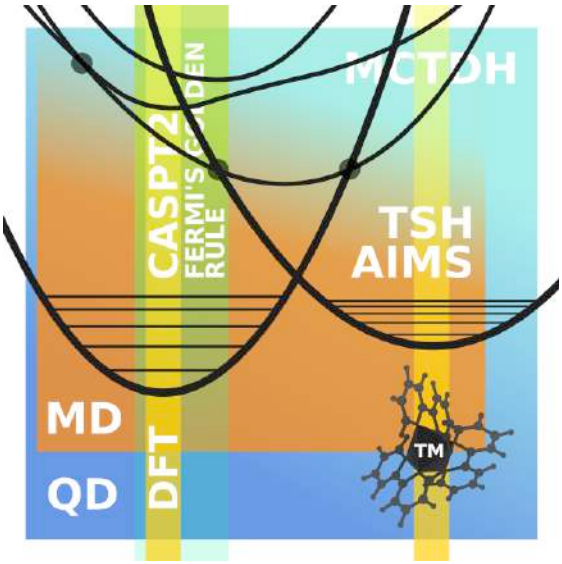
Behaviour of the curve GAD-CD (blue) on a PES. The set of arrows (green) shows the evolution of the control vectors.

An algorithm to locate transition states on a potential energy surface (PES) was proposed and described. The technique is based on the gentlest-ascent-dynamics (GAD) method where the gradient of the PES is projected into a given direction and also perpendicular to it. In the proposed method, named GAD-conjugate-direction (GAD-CD), the projection is not only applied to the gradient but also to the Hessian matrix. Then, the resulting Hessian matrix is block diagonal. The direction is updated according to the GAD method. Furthermore, to ensure stability and to avoid a high computational cost, a trust region technique is incorporated and the Hessian matrix is updated at each iteration. The performance of the algorithm in comparison with the standard ascent dynamics is discussed for a simple two-dimensional model PES. Its efficiency for describing the reaction mechanisms involving small and medium size molecular systems is demonstrated for molecular systems of interest in chemistry.

Deactivation of excited states in transition metal complexes: Insight from computational chemistry.

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

Chem. Eur. J. 25 (2019) 1152-1164.



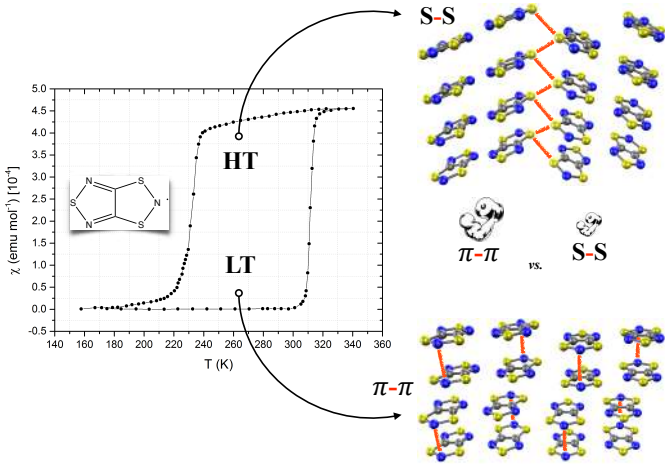
State of the art computational methodologies to study the excited-state decay dynamics in transition metal materials.

Investigation of the excited state decay dynamics of transition-metal systems is a crucial step for the development of photoswitchable molecular based materials with applications in growing fields as energy conversion, data storage, or molecular devices. An overview is presented of the state-of-the-art methodologies available to address the several aspects that have to be incorporated to properly describe the deactivation of excited states in transition-metal complexes.

Reorganization of intermolecular interactions in the polymorphic phase transition of a prototypical dithiazolyl-based bistable material.

T. Francese, F. Mota, M. Deumal, J. J. Novoa, R. W. A. Havenith, R. Broer, J. Ribas-Arino.

Cryst. Growth Des., *19* (2019) 2329.

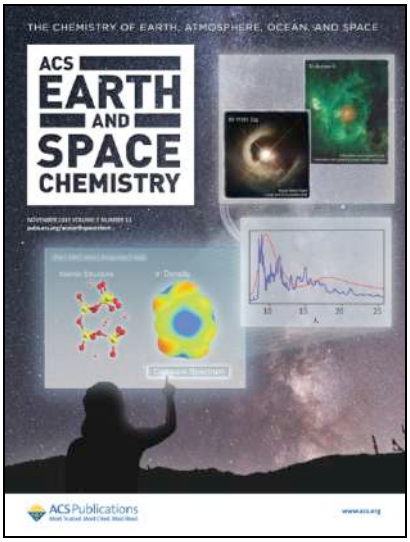


The spin transitions undergone by several molecular crystals of dithiazolyl (DTA) radicals make this type of radical promising candidates for future sensors and memory devices. In this work, we performed a systematic computational study of the intermolecular interactions existing in the two polymorphs of the neutral radical 1,3,5-trithia-2,4,6- triazapentalenyl in order to elucidate the origin of the difference in energy between those two polymorphs involved in its spin transition and to understand the crystal packing of this prototype of bistable materials. The π−π interactions between radicals are the main driving force for the crystal packing of both polymorphs, which comprises π-stacks of radicals. The difference in energy between polymorphs, in turn, is mainly controlled also by the intrastack π−π intermolecular interactions, and the interstack S···S contacts. Since the supramolecular motifs herein identified as important for the crystal packing and/or for the energy difference between polymorphs (and, thus, for the spin transition temperature) are common to other members of the DTA family, our results provide valuable information to understand better the structure and properties of other switchable DTA-based materials.

Structure and properties of nanosilicates with olivine $(Mg_2SiO_4)_N$ and pyroxene $(MgSiO_3)_N$ compositions.

A. Macia Escatllar, T. Lazaukas, S. M. Woodley, S. T. Bromley.

ACS Earth Space Chem., *3* (2019) 2390-2403.

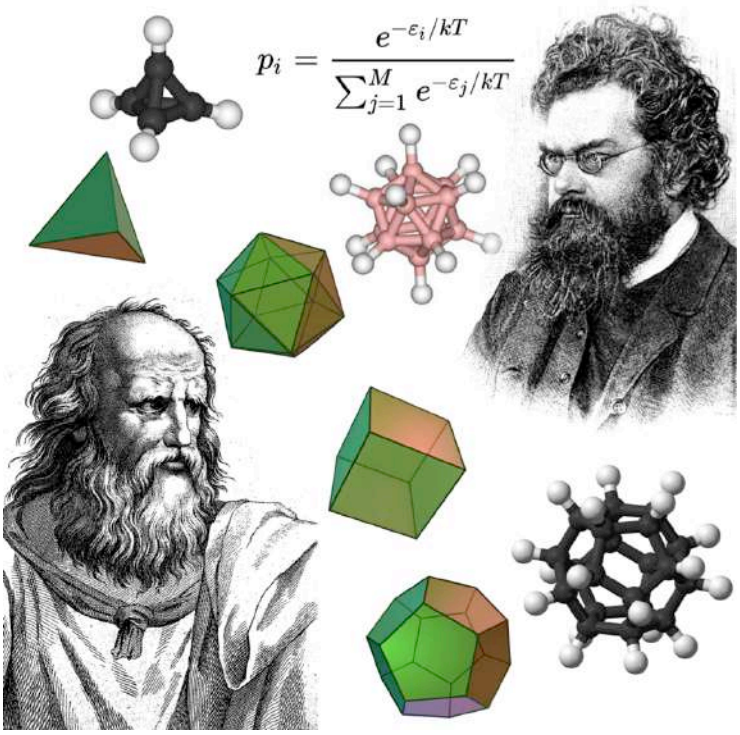


Magnesium-rich silicates are ubiquitous both terrestrially and astronomically, where they are often present as small particles. Nanosized Mg-rich silicate particles are likely to be particularly important for understanding the formation, processing, and properties of cosmic dust grains. Overall, our work provides a new platform for an accurate and detailed understanding of nanoscale silicates.

Effects of temperature on the shape and symmetry of molecules and solids.

A. Carreras, E. Bernuz, X. Marugan, M. Llunell, P. Alemany.

Chem. Eur. J. *25* (2019) 673-691.



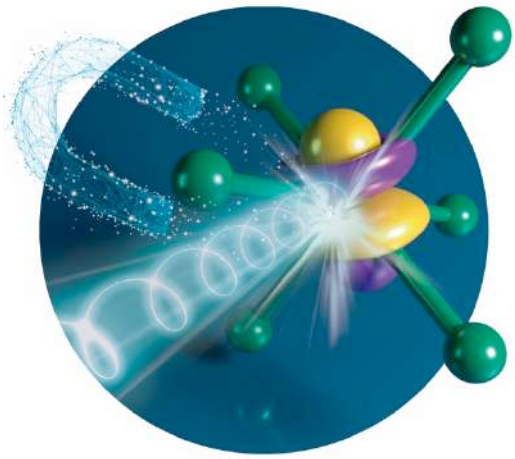
How does temperature change the shape of molècules? Bridging the gaps between Plato and Boltzman using continuous shape measures.

Despite its undeniable problems from a philosophical point of view, the concept of molecular structure, with attributes such as shape and symmetry, directly borrowed from the description of macroscopic objects, is nowadays central to most of chemistry. Following this trend, descriptions such as "the tetrahedral" carbon atom are widely used from elementary textbooks to the most up-to-date research articles. The definition of molecular shape is, however, not as simple as it might seem at first sight. Molecules don't behave as macroscopic objects do due to the incessant motion of its constituent particles, nuclei and electrons. How are molecular shape and symmetry affected by this thermal motion? In this review we introduce the language of continuous symmetry measures as a new tool to quantitatively describe the effects of temperature on molecular shape and symmetry.

$[UF_6]^{2-}$: A molecular hexafluorido actinide(IV) complex with compensating spin and orbital magnetic moments.

K. S. Pedersen, K. R. Meihaus, A. Rogalev, F. Wilhelm, D. Aravena, M. Amoza, E. Ruiz, J. R. Long, J. Bendix, R. Clérac.

Angew. Chem. Int. Ed. *58* (2019) 15650**.**



Cartoon that symbolizes the combination of computational and experimental studies on a novel uranium anion.

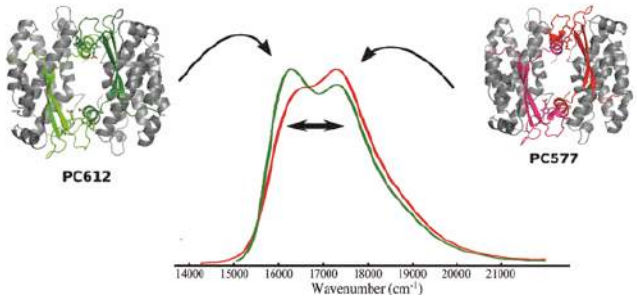
Synthesis, structural determination and spectroscopic and magnetic studies of a novel uranium anion, carried out by an international team in which two researchers from the IQTC were in charge of the multireference CASSCF calculations that allow to explain the unexpectedly very small magnetization found in synchrotron XMCD (X-ray magnetic circular dichroism) measurements as due to the compensation of spin and orbital contributions.

LINE 3. BIOMEDICINE AND SOFT MATTER

Spectral variability in phycocyanin cryptophyte antenna complexes is controlled by changes in the α polypeptide chains.

M. Corbella, L. Cupellini, F. Lipparini, G. D. Scholes, C. Curutchet.

ChemPhotoChem, *3* (2019) 945.



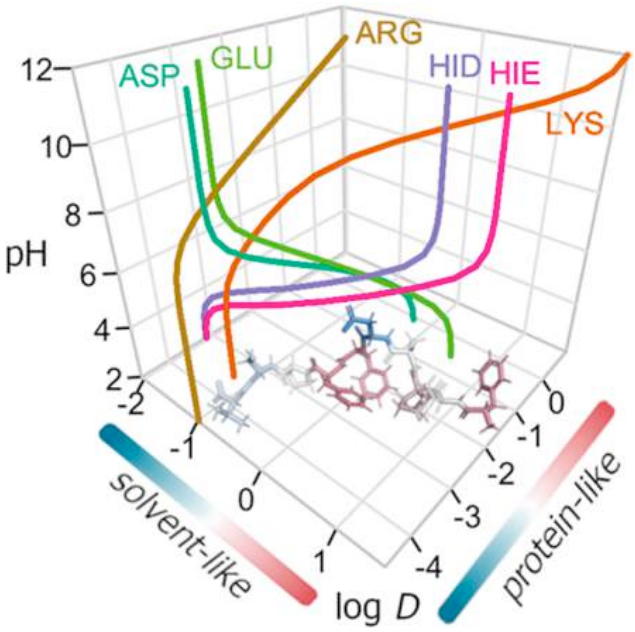
Multiscale simulations indicate that differences in the light harvesting properties of the PC577, PC612, PC630 and PC645 cryptophyte antenna complexes arise from changes in the α polypeptide chains in the structure.

Quantitative models of light harvesting in photosynthetic antenna complexes depend sensitively on the challenging determination of the relative site energies of the pigments. This study analyzed the basis of the light harvesting properties of four antennae from cryptophyte algae (PC577, PC612, PC630 and PC645), which have attracted much attention due to the recent observation of coherence effects in their light-harvesting mechanisms. By using multiscale polarizable quantum/molecular mechanics (QM/MMPol) calculations, it demonstrates that these four proteins share a common energetic ordering PCB82 < PCB158 < DBV51/61 for pigments located in the highly-conserved β chains, whereas bilins in the more divergent α chains cause their spectral differences. Moreover, the study provides a solid excitonic Hamiltonian of these proteins that paves the way for a detailed analysis of the basis supporting the coherence effects observed in their energy transport processes.

Development of a structure-bsed pH-dependent lipophilicity scale of amino acids from continuum solvation calculations.

W. J. Zamora, J. M. Campanera, F. J. Luque.

J. Phys. Chem. Letters., *10* (2019) 883.



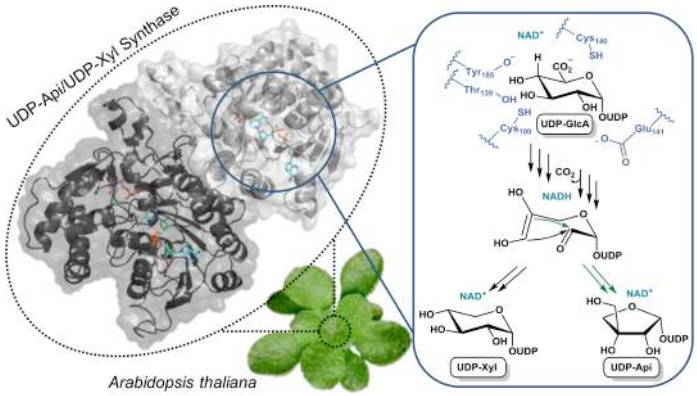
Representation of the logD of selected amino acids in the two hydrophobicity scales.

We report a versatile strategy to derive a pH-adapted scale that relies on theoretical estimates of distribution coefficients from conformational ensembles of amino acids. This is accomplished by using an accurately parametrized version of the IEFPCM/MST continuum solvation model as an effective way to describe the partitioning between n-octanol and water, in conjunction with a formalism that combines partition coefficients of neutral and ionic species of residues and the corresponding pKa values of ionizable groups. Two weighting schemes are considered to derive solvent-like and protein-like scales, which have been calibrated by comparison with other experimental scales developed in different chemical/biological environments and pH conditions as well as by examining properties such as the retention time of small peptides and the recognition of antigenic peptides. A straightforward extension to nonstandard residues is enabled by this efficient methodological strategy.

Deciphering the enzymatic mechanism of sugar ring contraction in UDP-apiose biosynthesis.

S. Savino, A. J. E. Borg, A. Dennig, M. Pfeiffer, F. de Giorgi, H. Weber, K. D. Dubey, C. Rovira, A. Mattevi, B. Nidetzky.

Nat. Catal., *2* (2019) 1115.

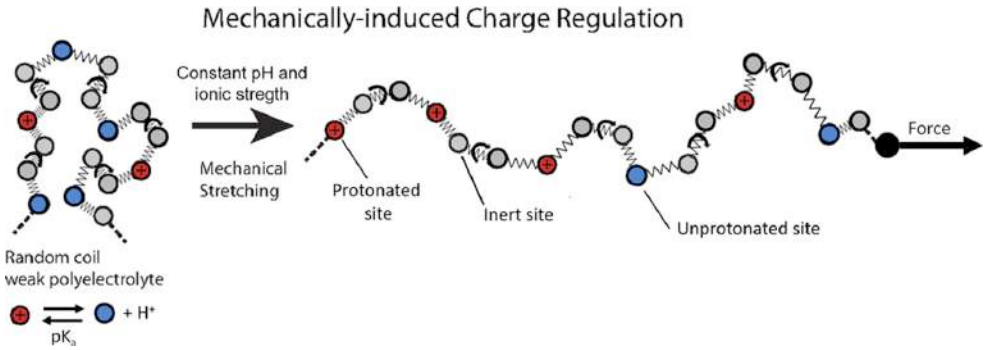


In changing weather situations, plants need to be robust and flexible at the same time. These structural properties are anchored the cell walls, which are largely built from polymers and polysaccharides. As binding agents, polysaccharides have the important task to connect long-chain polymers and to build a molecular network of tiny strands, called fibrils, which contribute to the tensile strength of the plant. One of the sugar building blocks is the branched-chain monosaccharide apiose. The mechanism responsible for apiose production of in nature was still unknown. Recently it has been discovered how apiose is produced by a single enzyme called UAXS (UDP-apiose/UDP-xylose Synthase) and the entire mechanism of this enzyme has been decoded by an interdisciplinary collaboration. The UAXS-enzyme selectively catalyzes four reaction steps, resulting in the change from a six ring sugar molecule (hexose) to a structural converted five ring sugar (pentose). By creating new organic carbon compounds, the enzyme is responsible for giving plants their strength properties.

Effect of charge regulation and conformational equilibria in the stretching properties of weak polyelectrolytes.

P. M. Blanco, S. Madurga, F. Mas, J. L. Garcés.

Macromolecules *52* (2019) 8017-8031.



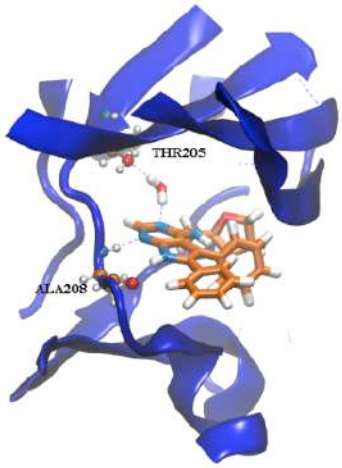
Scheem of a weak polyelectrolyte model under the influence of pH, ionic strength and external force. Monomers are represented as sites joined by flexible harmonic bonds.

Weak polyelectrolytes can modulate their charge in response to external perturbations, such as changes in the pH, ionic strength (I), or electrostatic interactions with other charged species, a phenomenon known as charge regulation (CR). On the other hand, it is well established that CR is highly coupled with the conformational degrees of freedom. In this paper, the influence of CR in the stretching properties of weak polyelectrolytes is analyzed, and the possibility of CR induced by mechanical stretching is explored. With this aim, we make use of a minimal model, which captures the fundamental aspects present in the stretching of a flexible weak linear polyelectrolyte: internal angle rotation, bond stretching, bond bending, and proton binding, which is the paradigmatic mechanism of CR. Mechanical stretching is studied by performing semi-grand canonical Monte Carlo simulations at different pH and ionic strength conditions.

Effect of set up protocols on the accuracy of alchemical free energy calculation over a set of ACK1 inhibitors.

J. M. Granadino-Roldán, A. S. J. S. Mey, J. J. Pérez González, S. Bosisio, J. Rubio-Martinez, J. Michel.

PLoS ONE *14* (2019) e0213217.



Snapshot taken after 2 ns of MD showing the manually placed water molecule inside the ATP-binding pocket.

Hit-to-lead virtual screening frequently relies on a cascade of computational methods that starts with rapid calculations applied to a large number of compounds and ends with more expensive computations restricted to a subset of compounds that passed initial filters. This work focuses on set up protocols for alchemical free energy (AFE) scoring in the context of a Docking – MM/PBSA – AFE cascade.

III.2 PUBLICATION LIST

PUBLISHED ARTICLES

1. *$La_{1.5}Sr_{0.5}NiMn_{0.5}Ru_{0.5}O_6$ double perovskite with enhanced ORR/OER bifunctional catalytic activity.*
M. Retuerto, F. Calle-Vallejo, L. Pascual, G. Lumbeeck, M. Fernández-Díaz, M. Croft, J.Gopalakrishnan, M. A. Peña, J. Hadermann, M. Greenblatt, S. Rojas.
ACS Appl. Mater. Inter. *11* (2019) 21454-21464.

2. *Molecular mechanisms of oxygen activation and hydrogen peroxide formation in lytic polysaccharide monooxygenases.*
B. Wang, P. H. Walton, C. Rovira.
ACS Catal. *9* (2019) 4958-4969.

3. *Adsorption preference determines segregation direction: a shortcut to more realistic surface models of alloy catalysts.*
S. Liu, Z.-J. Zhao, C. Yang, S. Zha, K. M. Neyman, F. Studt, J. Gong.
ACS Catal. *9* (2019) 5011-5018.

4. *Kinetic Monte Carlo simulations unveil synergic effects at work on bifunctional catalysts.*
H. Prats, S. Posada-Pérez, J. A. Rodríguez, R. Sayós, F. Illas.
ACS Catal. *9* (2019) 9117-9126.

5. *Outlining the scaling-based and scaling-free optimization of electrocatalysts.*
N. Govindarajan, M. T. M. Koper, E. J. Meijer, F. Calle-Vallejo.
ACS Catal. *9* (2019) 4218-4225.

6. *Dynamic and functional profiling of xylan-degrading enzymes in Aspergillus secretomes using activity-based probes.*
S. Schröder, C. de Boer, Casper, N. McGregor, R. Rowland, O. Moroz, E. Blagova, J. Reijngoud, M. Arentshorst, D. Osborn, M. Morant, E. Abbate, M. Stringer, K. Krogh, L. Raich, C. Rovira, J.-G. Berrin, G. van Wezel, A. Ram, B. Florea, G. A. van der Marel, J. Codée, K. Wilson, L. Wu, G. J. Davies, H. S. Overkleeft.
ACS Cent. Sci. *5* (2019) 1067-1078.

7. *What can infrared spectra tell us about the crystallinity of nanosized interstellar silicate dust grains?*
L. Zamirri, A. Macia Escatllar, J. Marinoso Guiu, P. Ugliengo, S. T. Bromley.
ACS Earth Space Chem. *3* (2019) 2323-2338.

8. *Structure and properties of nanosilicates with olivine $(Mg_2SiO_4)_N$ and pyroxene $(MgSiO_3)_N$ compositions.*
A. Macia Escatllar, T. Lazaukas, S. M. Woodley, S. T. Bromley.
ACS Earth Space Chem. *3* (2019) 2390-2403.

9. *Oxidative cleavage of cellobiose by lytic polysaccharide monooxygenase (LPMO)-inspired copper complexes.*
A. C. Neira, P. R. Martínez-Alanis, G. Aullón, M. Flores-Alamo, P. Zerón, A. Company, J. Chen, J. B. Kasper, W. R. Browne, E. Nordlander, I. Castillo.
ACS Omega *4* (2019) 10729-10740.

10. *Subsurface carbon – a general feature of noble metals.*
O. Piqué, I. Z. Koleva, F. Viñes, H. A. Aleksandrov, G. N. Vayssilov.
Angew. Chem. Int. Ed. *58* (2019) 1744-1748.

11. *Enhanced electroreduction of carbon dioxide to methanol using zinc dendrites pulse-deposited on silver foam.*
Q. H. Low, N. W. X. Loo, F. Calle-Vallejo, B. S. Yei.
Angew. Chem. Int. Ed. *58* (2019) 2256-2260.

12. *The periodic table – a universal icon: its birth 150 years ago, and its popularization through literature, art and music.*
S. Shaik, E. Cremades, S. Alvarez.
Angew. Chem. Int. Ed. *58* (2019) 13194-13206.

13. *Electrochemically gated long distance charge transport in photosystem.*
M. López-Martínez, M. López-Ortiz, M. E. Antinori, E. Wientjes, A. Nin-Hill, C. Rovira, R. Croce, I. Díez-Pérez, P. Gorostiza.
Angew. Chem. Int. Ed. *58* (2019) 13280-13284.

14. *$[UF6]^{2-}$: A molecular hexafluorido actinide(IV) complex with compensating spin and orbital magnetic moments.*
K. S. Pedersen, K. R. Meihaus, A. Rogalev, F. Wilhelm, D. Aravena, M. Amoza, E. Ruiz, J. R. Long, J. Bendix, R. Clerac.
Angew. Chem. Int. Ed. *58* (2019) 15650-15654.

15. *A proposal for evading the measurement uncertainty in classical and quantum computing: application to a resonant tunneling diode and a Mach-Zehnder interferometer.*
D. Pandey, L. Bellentani, M. Villani, G. Albareda, P. Bordone, A. Bertoni, X. Oriols.
Appl. Sci. *9* (2019) 2300-2320.

16. *Pharmacology and preclinical validation of a novel anticancer compound targeting PEPCK-M.*
M. Aragó, J. Moreno-Felici, S. Abás, S. Rodríguez-Arévalo, P. Hyrossová, A. Figueras, F. Viñals, B. Pérez, M. I. Loza, J. Brea, P. Latorre, J. A. Carrodeguas, P. M. García-Rovés, C. Galdeano, T. Ginex, F. J. Luque, C. Escolano, J. C. Perales.
Biomed. Pharmacother. *121* (2019) 109601.

17. *A photoswitchable GABA receptor channel blocker.*
G. Maleeva, D. Wutz, K. Rustler, A. Nin-Hill, M. Alfonso-Prieto, E. Petukhova, A. Bautista-Barrufet, A. Gomila-Juaneda, P. Scholze, F. Peiretti, C. Rovira, B. König, P. Gorostiza, P. Bregestovski.
Br. J. Pharmacol. *176* (2019) 2661-2677.

18. *Nickel-catalyzed aryl trifluoromethyl sulfides synthesis: a DFT study.*
J. Jover.
Catal. Sci. Technol. *9* (2019) 5962-5970.

19. *Synthesis, characterization, solution behavior and theoretical studies of Pd(II) allyl complexes with 2-phenyl-3H-indoles as ligands.*
M. Tomé, A. Grabulosa, M. Rocamora, G. Aullón, T. Calvet, M. Font-Bardía, C. López.
Catalysts *10* (2019) 811.

20. *Conformational effects of $[Ni_2(\mu\text{-}SAr)_2]$ cores on their electrocatalytic activity.*
A. Mondragón-Díaz, E. Robles-Marín, B. A. Murueta-Cruz, J. C. Aquite, P. R. Martínez-Alanis, M. Flores-Alamo, G. Aullón, L. N. Benítez, I. Castillo.
Chem. Asian J. *14* (2019) 3301-3312.

21. *Slow-spin relaxation of a low-spin S = 1/2 Fe^{III} carborane complex.*
A. B. Buades, V. S. Arderiu, L. Maxwell, M. Amoza, D. Choquesillo-Lazarte, N. Aliaga-Alcalde, C. Viñas, F. Teixidor, E. Ruiz.
Chem. Commun. *55* (2019) 3825-3828.

22. *Open-shell jellium aromaticity in metal clusters.*
J. Poater, M. Solà.
Chem. Commun. *55* (2019) 5559-5562.

23. *Assessing the usefulness of transition metal carbides for hydrogenation reactions.*
H. Prats, J. J. Piñero, F. Viñes, S. T. Bromley, R. Sayós, F. Illas.
Chem. Commun. *55* (2019) 12797-12800.

24. *Pressure selection for non-reactive and reactive pressure-swing distillation.*
A. Risco, V. Plesu, J. A. Heydenreich, J. Bonet, A. E. Bonet-Ruiz, A. Calvet, P. Iancu, J. Llorens.
Chem. Eng. Process. - Process Intensification *135* (2019) 9-21.

25. *Castor oil biorefinery: conceptual process design, simulation and economic analysis.*
A. C. Dimian, P. Iancu, V. Plesu, A. E. Bonet-Ruiz, J. Bonet-Ruiz.
Chem. Eng. Res. Des. *141* (2019) 198-219.

26. *Hydration of cyclohexene to cyclohexanol in a hybrid reactive distillation with a side decantar.*
I. Marchante, A. E. B. Ruiz, V. Plesu, J. Bonet-Ruiz, P. Iancu, J. Llorens.
Chem. Eng. Trans. *76* (2019) 25-30.

27. *Integrated reaction-separation processes sequencing and screening at early stages of design.*
K. Marin, J. Bonet-Ruiz, A. E. Bonet-Ruiz, V. Plesu, P. Iancu, J. Llorens.
Chem. Eng. Trans. *76* (2019) 631-636.

28. *Deactivation of excited states in transition metal complexes: Insight from computational chemistry.*
C. Sousa, M. Alías, A. Domingo, C. de Graaf.
Chem. Eur. J. *25* (2019) 1152-1164.

29. *Effects of temperature on the shape and symmetry of molecules and solids.*
A. Carreras, E. Bernuz, X. Marugan, M. Llunell, P. Alemany.
Chem. Eur. J. *25* (2019) 673-691.

30. *Ammonia–borane derived BN fragments trapped on bi- and trimetallic titanium(III) systems.*
E. del Horno, J. Jover, M. Mena, A. Pérez-Redondo, C. Yélamos.
Chem. Eur. J. *25* (2019) 7096-7100.

31. *Magnetization slow dynamics in ferrocenium complexes.*
M. Ding, A. K. Hickey, M. Pink, J. Telser, D. L. Tierney, M. Amoza, M. Rouzieres, T. J. Ozumerzifon, W. A. Hoffert, M. P. Shores, E. Ruiz, R. Clerac, J. M. Smith.
Chem. Eur. J. *25* (2019) 10625-10632.

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E. Gianquinto, I. Moscetti, O. De Bei, B. Campanini, M. Marchetti, F. J. Luque, S. Cannistraro, L. Ronda, A. R. Bizzarri, F. Spyrakis, S. Bettati.
Sci. Rep. *9* (2019) 18629.

128. *Silver atom, trimer and tetramer species supported on a ceria nanoparticle: a density functional study.*
V. A. Nasluzov, E. A. Ivanova-Shor, A. M. Shor, K. M. Neyman.
Surf. Sci. *681* (2019) 38-46.

129. *Study of active surface centers of Pt/CeO_2 catalysts prepared using radio-frequency plasma sputtering technique.*
A. I. Stadnichenko, V. V. Muravev, S. V. Koscheev, V. I. Zaikovskii, H. A. Aleksandrov, K. M. Neyman, A. I. Boronin.
Surf. Sci. *679* (2019) 273-283.

130. *Differential many-body effects for initial and core-ion states: impact on XPS spectra.*
P. S. Bagus, C. Sousa, F. Illas.
Theor. Chem. Acc. *138* (2019) 61.

131. *Electronic energy transfer in biomacromolecules.*
L. Cupellini, M. Corbella, B. Mennucci, C. Curutchet.
WIREs Comput. Mol. Sci. *9* (2019) e1392.

BOOK CHAPTERS AND PROCEEDINGS

1. *150 Anys de Taules Periòdiques a la UB.*
   edited by S. Alvarez and C. Mans (Edicions UB, Barcelona) 2019.

2. *100 Curiositats sobre la Taula Periòdica i els elements químics.*
   S. Alvarez, author of some chapters.
   coedited by S. Alvarez (Ed. Cossetània, Valls) 2019. ISBN: 978-84-9034-844-4.

3. *How to design models for ceria nanoparticles: challenges and strategies for describing nanostructured reducible oxides.*
   A . Bruix, K.M. Neyman.
   Computational Modelling of Nanoparticles, vol. 12, p. 55-99 (series: Frontiers of Nanoscience) edited by S. T. Bromley and S. M. Woodley (Elsevier, Oxford) 2019.

4. *Fractal Dimension (FD).*
   P. M. Blanco, S. Madurga, A. Isvoran, L. Pitulice, F. Mas.
   New Frontiers in Nanochemistry. Concepts, Theories, and Trends, vol. 1, cap. 16, p. 171-186 (series: Structural Nanochemistry) edited by M. V. Putz (Apple Academic Press, EUA) 2019.

5. *Fractal Kinetics (FK).*
   F. Mas, L. Pitulice, S. Madurga, J. L. Garcés, E. Vilaseca, A. Isvoran.
   New Frontiers in Nanochemistry. Concepts, Theories, and Trends, vol. 1, cap. 17, p. 187-199 (series: Structural Nanochemistry) edited by M. V. Putz (Apple Academic Press, USA) 2019.

6. *Macromolecular Crowding (MC).*
   A. Isvoran, L. Pitulice, E. Vilaseca, I. Pastor, S. Madurga, F. Mas.
   New Frontiers in Nanochemistry. Concepts, Theories, and Trends, vol. 3, cap. 20, p. 307-317 (series: Sustainable Nanochemistry) edited by M. V. Putz (Apple Academic Press, USA) 2019.

7. *Simulation paths of anticancer drugs on a graphene oxide surface.*
   M. Nedyalkova, J. Romanova, J. Stoycheva, S. Madurga.
   Graphene Functionalization Strategies. From Synthesis to Applications, p. 215-228 edited by A. Khan, M. Jawaid, B. Neppolian and A. Asiri (Ed. Springer, Singapore) 2019.

III.3 OTHER ACTIVITIES

PHD THESES 2019

1. *Toward refined theoretical models for the description of lipophilicity in biomolecules.*
   William J. Zamora
   PhD program: Biotechnology.
   Faculty of Pharmacy and Food Sciences, University of Barcelona.
   Supervisor/s: F. J. Luque, J. M. Campanera.
   February 2019

2. *Rationalization of the mechanism of bistability in dithiazolyl-based molecular magnets.*
   Tommaso Francese
   PhD program: Theoretical Chemistry and Computational Modelling.
   Faculty of Chemistry, University of Barcelona.
   Supervisor/s: J. J. Novoa Vide, Ria Broer.
   March 2019.

3. *Monte Carlo based methods applied to heterogeneous catalysis and gas separation.*
   Héctor Prats García
   PhD program: Theoretical Chemistry and Computational Modelling.
   Faculty of Chemistry, University of Barcelona.
   Supervisor/s: Ramón Sayós, Francesc Illas.
   March 2019.

4. *Desarrollos metodológicos en la exploración de la especie bioactiva en fármacos: Búsqueda de agentes antimaláricos.*
   Antonio Viayna Gaza
   PhD program: Biotechnology.
   Faculty of Pharmacy and Food Sciences, University of Barcelona.
   Supervisor/s: F. J. Luque.
   June 2019.

5. *On the usage of lipophilic descriptors for molecular similarity evaluation.*
   Javier Vázquez Lozano
   PhD program: Biotechnology.
   Faculty of Pharmacy and Food Sciences, University of Barcelona.
   Supervior/s: F. J. Luque, Enric Herrero.
   September 2019.

6. *Models and computational methods applied to industrial gas separation processes and enhanced oil recovery.*
Gerard Alonso Benito
PhD program: Theoretical Chemistry and Computational Modelling.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: Ramón Sayós, Pablo Gamallo.
November 2019.

7. *Anisotropía en imanes unimoleculares y qubits con complejos metálicos con espín S = 1/2.*
Martín Amoza Dávila
PhD program: Molecular Inorganic Chemistry.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: E. Ruiz.
November 2019.

8. *Theoretical reaction and relaxation dynamics in superfluid helium nanodroplets.*
Miquel Blancafort Jorquera
PhD program: Theoretical Chemistry and Computational Modelling.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: Miguel González.
November 2019.

9. *The supramolecular organization of cancer metabolism: from macromolecular crowding to metabolic reprograming underlyng cancer metastasis and drug resistance.*
Cristina Balcells Nadal
PhD program: Molecular Biotechnology.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: Marta Cascante, Francesc Mas.
December 2019.

MASTER THESES 2019

1. *Simulation and experimental struvite crystallization with real waste water.*
   Víctor Alcaraz Esteban
   MSc program: Chemical Engineering.
   Faculty of Chemistry, University of Barcelona.
   Supervisor/s: Alexandra Plesu Popescu, Joan Llorens Llacuna.
   February 2019.

2. *CFD Analysis of mass transfer, shear stress and hydrodynamics in a lab apparatus to test forward osmosis membranes.*
   Álex Terradillos Guillén
   MSc program: Chemical Engineering.
   Faculty of Chemistry, University of Barcelona.
   Supervisor/s: Alexandra Plesu Popescu, Joan Llorens Llacuna.
   April 2019.

3. *CFD study of NOx emissions decreases by flame additives.*
   Hector Joel López Molina
   MSc program: Chemical Engineering.
   Faculty of Chemistry, University of Barcelona.
   Supervisor/s: Alexandra Plesu Popescu, Jordi Bonet i Ruiz.
   April 2019.

4. *Optimization of ethanol and ethyl acetate separation by pressure swing distillation.*
   Víctor Manso Álvarez
   MSc program: Chemical Engineering.
   Faculty of Chemistry, University of Barcelona.
   Supervisor/s: Alexandra Plesu Popescu, David Curcó Cantarell.
   April 2019.

5. *Insights on Mo activity in deoxygenation reactions.*
   Biel Martínez Díaz
   MSc program: Theoretical Chemistry and Computational Modelling.
   Faculty of Chemistry, University of Barcelona.
   Supervisor/s: Francesc Viñes.
   June 2019.

6. *A novel intensified process for bioethanol dehydration and blending.*
   José Luis Pellín Moreno
   MSc program: Chemical Engineering.
   Faculty of Chemistry, University of Barcelona.
   Supervisor/s: Alexandra Plesu Popescu, Manuel Vicente Buil.
   June 2019.

7. *CFD Modelling with MFIX® of liquid-solid fluidized beds of polydisperse struvite crystals.*
Ricardo Moya Chamizo
MSc program: Chemical Engineering.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: Alexandra Plesu Popescu, Ricard Torres Castillo.
June 2019.

8. *Water cycle management and indicators: a review.*
Aitor Barroso Roig
MSc program: Environmental Engineering.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: Alexandra Plesu Popescu, Jordi Bonet i Ruiz.
June 2019.

9. *Surrogate model for chemical absorbents mixtures for CO_2 capture.*
Enric Selfa Martínez
MSc program: Environmental Engineering.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: Alexandra Plesu Popescu, Jordi Bonet i Ruiz.
June 2019.

10. *ANSYS Fluent simulation of a conventional chimney.*
Roger Pitarch Gres
MSc program: Environmental Engineering.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: Alexandra Plesu Popescu, Ricard Torres Castillo.
June 2019.

11. *Comprehensive study of carbon dioxide hydrogenation over Ni (111) surface: reverse Water-Gas Shift reaction vs. Sabatier reaction.*
Pablo Lozano-Reis
MSc program: Theoretical Chemistry and Computational Modelling.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: Pablo Gamallo, Ramón Sayós.
July 2019.

12. *Unravelling calmodulin conformational ensemble from combined molecular dynamics and FRET simulations.*
Daniel Gonzalo Palao
MSc program: Environmental Engineering.
Faculty of Pharmacy and Food Sciences, University of Barcelona.
Supervisor/s: Carles E. Cuturchet.
July 2019.

13. *Study of the transglycosylation complex of β - galactosidase using molecular dynamics.*
Iker Zapiráin Gysling
MSc program: Theoretical Chemistry and Computational Modelling.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: Carme Rovira.
July 2019.

14. *Theoretical insight into the active site dynamics of fucosyltransferases.*
Beatriz Piniello Castillo
MSc program: Atomistic and Multiscale Computational Modelling in Physics, Chemistry and Biochemistry.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: Carme Rovira.
July 2019.

15. *Disociación de CO_2 catalizada por MXenes.*
Raul Morales Salvador
MSc program: Atomistic and Multiscale Computational Modelling in Physics, Chemistry and Biochemistry.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: Ángel Morales-García, Francesc Viñes.
July 2019.

16. *First-principles evaluation of the initial oxidation of transition metal surfaces.*
Anabel Jurado Mañas
MSc program: Chemistry of Advanced Materials.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: Francesc Viñes.
July 2019.

17. *Relacions estructura/propietats magnètiques a la unitat $[Dy_2(RCOO)_4]$.*
Alba Palacios Requena
MSc program: Theoretical Chemistry and Computational Modelling.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: Jordi Cirera.
July 2019.

18. *Desenvolupament d'un camp de forces per primers principis per a gàbies metal·lo-orgàniques de $[Fe_4]$.*
Laia Navarro Maestro
MSc program: Atomistic and Multiscale Computational Modelling in Physics, Chemistry and Biochemistry.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: Jordi Cirera.
July 2019.

19. *Quantum chemical examination of the influence of substituents on the spin crossover temperature of manganocenes.*
Florian Matz
Faculty of Chemistry, University of Barcelona & Institut für Physikalische Chemie und Elektrochemie (Hannover, Germany).
Supervisor/s: Jordi Cirera.
July 2019.

20. *Setting up a methodology to decipher cryptic pockets.*
Pol Costas Viñas
MSc program: Theoretical Chemistry and Computational Modelling.
Faculty of Sciences, Autonomous University of Madrid.
Supervisor/s: Jaime Rubio Martínez.
July 2019.

21. *Selective allosteric inhibition of TKTL1 protein.*
Kassiani Motaki
MSc program: Theoretical Chemistry and Computational Modelling.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: Jaime Rubio Martínez.
July 2019.

22. *Quest for compounds that selectively activate the pro-apoptotic Bax protein.*
Natàlia de Moya Valenzuela
MSc program: Theoretical Chemistry and Computational Modelling.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: Jaime Rubio Martínez.
July 2019.

23. *Chemical ordering in Ag-Pt nanoalloys: structures and spectra.*
Sofia Olobardi
MSc program: Chemistry.
Dipartimento di Scienze Chimiche e Farmaceutiche, Università di Trieste, Italy.
Supervisor/s: Mauro Stener, Konstantin Neyman.
July 2019.

24. *New computational strategies to obtain kinetic data of enzymatic processes in crowded media.*
Raquel Agraso Riobó
MSc program: Atomistic and Multiscale Computational Modelling in Physics, Chemistry and Biochemistry.
Faculty of Chemistry, University of Barcelona.
July 2019.

25. *How to accurately model the IR spectra of cosmic nanosilicate dust grains.*
Joan Mariñoso Guiu
MSc program: Theoretical Chemistry and Computational Modelling.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: Stefan T. Bromley.
July 2019.

26. *Modelling lacto-n-biosidase from Bifidobacterium bifidum by means of molecular dynamics.*
Irene Cuxart Sánchez
MSc program: Bioengineering.
Institut Químic de Sarrià, Ramon Llull's University.
Supervisor/s: Carme Rovira.
September 2019.

SCIENTIFIC CONFERENCES AND MEETINGS 2019

Scientific Advisory Board Meeting of the MPSD
Hamburg (Germany) 9 January 2019

Trajectory Approaches for Nonequilibrium Quantum Dynamics in Light-Matter Systems (poster)
G. Albareda, A. Kelly, H. Appel, S. Sato, K. Lively, C. Schaffer, N. Hoffmann, A. Rubio

10th Symposium on Computing π-Conjugated Compounds
Valencia (Spain) 31 January – 2 February 2019

Understanding spectral variability in cryptophyte antenna complexes from multiscale simulations (oral communication)
C. Curutchet

Chemistry Today for Tomorrow (Science and Education for Smart Growth)
Sofia (Bulgaria) 1 February 2019

New descriptions for proteins: separation of allergenic from non-allergenic proteins (oral communication)
S. Madurga, M. Nedyalkova, F. Mas, V. Simeonov

Modelling polyelectrolytes; coupling of conformational and ionization equilibria in solution (oral communication)
F. Mas, P. M. Blanco, S. Madurga, J. L. Garcés

Theoretical modeling of the transition temperature in spin-crossover molecules (oral communication)
J. Cirera

Spin transition in dithiazolyl based switchable materials (oral communication)
J. Ribas

Influence of charge regulation on conformational, ionization and stretching properties of polyelectrolytes (oral communication)
F. Mas, P. M. Blanco, S. Madurga, J. L. Garcés

Polymer-Borate hybrids films - Theoretical and experimental determination of the structure (poster)
H. Hristov, M. Nedyalkova, S. Madurga

Borosilicate hybrid materials and nanocomposites: synthetic, structural and statistical approach (poster)
H. Hristov, M. Nedyalkova, S. Madurga, V. Simeonov

Predicting partition coefficients by first principles calculations of organic solvents with implicit solvent model (poster)
M. Nedyalkova, S. Madurga, M. Tobiszewski, V. Simeonov

Presentació de l'Any Internacional de la Taula Periòdica
Barcelona (Spain) 5 February 2019

Presentació de peces musicals a l'Institut del Teatre (invited talk)
S. Alvarez

GrapheneforUS International Conference
New York (USA) 14-15 February 2019

CO_2 Chemical Trapping on Two-Dimensional MXenes (oral communication)
Á. Morales-García, F. Viñes, R. Morales-Salvador, F. Illas

Les mil cares de la taula periòdica (cicle de conferències de la Biblioteca de la Vila de Gràcia)
Barcelona (Spain) 18 February 2019

La taula periòdica com a referent cultural (invited talk)
S. Alvarez

APS Spring Meeting
Boston (USA) 4-8 March 2019

Room Temperature Magnetoresistance in Single-Molecule Device (invited talk)
E. Ruiz

Molecular Dynamics Today (MD2d)
Bologna (Italy) 14-15 March 2019

Toward a comprehensive understanding of the mechanisms of biological activity with molecular simulations (oral communication)
F. J. Luque

6th Computationally Driven Drug Discovery (CDDD) Meeting
Rome (Italy) 28-29 March 2019

On the Usage of Novel Hydrophobic Molecular Fields for CADD (oral communication)
A. DePlano, O. Rey, J. Vázquez, A. Herrero, E. Gibert, E. Herrero, F. J. Luque

ACS National Meetings
Orlando (USA) 31 March – 2 April 2019

Morphology Dependence of Stability and Properties of Stoichiometric TiO_2 Nanoparticles (oral communication)
Á. Morales-García, A. Macià, S. T. Bromley, F. Illas

CECAM School on Hybrid Quantum Mechanics / Molecular Mechanics (QM/MM) Approaches to Biochemistry and beyond
Lausanne (Switzerland) 8-12 April 2019

C. Rovira *(organization)*

CECAM School on Kinetics and Dynamics of Chemical Reactions
Zaragoza (Spain) 8-12 April 2019

P. Gamallo *(organization)*

Kinetic Monte Carlo Simulations (seminar)
P. Gamallo

Molecular Dynamics (seminar)
X. Giménez

Calculating kinetic coeficients of chemical reactions using quantum dynamics (seminar)
F. Huarte-Larrañaga

Wave-packet quantum Dynamics: overview and Applications to chemical reactions (seminar)
P. Gamallo

International Astronomical Union: S350 Laboratory Astrophysics
Cambridge (United Kingdom) 14 April 2019

Using Atomistically Detailed Simulations to Understand the Formation, Structure and Composition of Astrophysical Silicate Dust Grains (oral communication)
S. T. Bromley

Centre in Green Chemistry and Catalysis (CGCC) 10th Annual Symposium
Montreal (Canada) 11 May 2019

Insights in Mo_2C activity in deoxygenation reactions (poster)
B. Martínez, F. Viñes, P. McBreen, F. Illas

25th Topical Meeting of the International Society of Electrochemistry
Toledo (Spain) 12-15 May 2019

Why breaking scaling relations does not necessarily lead to better electrocatalysts (oral communication)
Federico Calle-Vallejo

FOTOFUEL Workshop on Solar Fuels
Madrid (Spain) 13-14 Maig 2019

Unbiased Analysis of the Interplay between Size, Morphology and Energy Gap in Realistic TiO_2 Nanoparticles (invited talk)
Á. Morales-García

13th Carbohydrate Bioengineering Meeting (CBM13)
Toulouse (France) 19 May 2019

Early stages of glycogen biosynthesis: mechanism of action of glycogenin (oral communication)
C. Rovira

Oxazoline or oxazolinium ion? The reaction mechanism of GH18 chitinases (oral communication)
J. Coines, M. Alfonso-Prieto, X. Biarnés, A. Planas, C. Rovira

World Chemistry Forum 2019
Barcelona (Spain) 22-24 May 2019

Novel catalysts for methane activation at room temperature (keynote talk)
F. Illas

Effects of oxide supports on reactivity of metal particles in catalysis and energy technologies (invited talk)
K. M. Neyman

XXXVII Reunión Bienal de la Real Sociedad Española de Química
Donostia (Spain) 26-30 May 2019

Multiscale modeling of light harvesting in cryptophyte photosynthesis (oral communication)
C. Curutchet

Games with the Periodic Table to increase public awareness of science (oral communication)
J. Poater, S. Simon, M. Miquel Solà, M. Duran

New Trends in Statistical Physics: 50 years of the Sitges Conference
Sitges (Spain) 27-31 May 2019

Weak Polyelectrolyte Modelling: Coupling Charge Regulation and Conformational Equilibria vis LEIP Methodology (poster)
J. L. Garcés, P. M. Blanco, S. Madurga, F. Mas

A New Model for Macromolecular Diffusion in Crowded Media: the Chain Entanglement Soft Potential (poster)
P. M. Blanco, S. Madurga, J. L. Garcés, F. Mas

MasterQuímica XV
Barcelona (Spain) 28-30 May 2019

Noves estartègies computacionals per obtenir dades cinètiques dels processos enzimàtics en medi aglomerat (poster)
R. Agraso, P. M. Blanco, S. Madurga, F. Mas

Theoretical Chemistry and Computational Modelling: 20 years promoting Excellence in Science (20TCCM)
Donostia (Spain) 30 May – 1 June 2019

Magnetic and Conductive properties in multifunctional bisdithiazolyl-based materials (oral communication)
C. Roncero

Bifunctional catalysts at work: unravelling synergic effects by kinetic Monte Carlo simulations (poster)
R. Sayós, H. Prats, S. Posada-Pérez, J. A. Rodriguez, F. Illas

X Simposium IQTC-UB
Barcelona (Spain) 31 Maig 2019

Jordi Cirera *(organization)*

A Computational View on Astronomical Silicate Nanoclusters (invited talk)
A. Macià

Mechanistic insights into substrate-assisted glycoside hydrolases (invited talk)
Joan Coines

Rotational relaxation in superfluid helium nanodroplets (poster)
M. Blancafort, A. Vilà, M. González

Vibrational relaxation in superfluid helium nanodroplets (poster)
M. Blancafort, A. Vilà, M. González

Unravelling Calmodulin conformational ensemble from combined Molecular Dynamics and FRET simulations (poster)
D. Gonzalo, C. Curutchet

Correcting Flaws in the Assignment of Nitrogen Chemical Environments in N-Doped Graphene (poster)
M. Figueras, I. J. Villar-Garcia, F. Viñes, C. Sousa, V. A. de la Peña O'Shea, F. Illas

Insights on Mo_2C Activity in Deoxygenation Reactions (poster)
B. Martínez, F. Viñes, P. McBreen, F. Illas

Carbon Dioxide Hydrogenation over Nickel Catalysts: DFT and Kinetic Monte Carlo (poster)
P. Lozano, H. Prats, P. Gamallo, F. Illas, R. Sayós

Accuracy of the Topological Approach for Nanoalloys: Case Study of PtCu Nanoparticles (poster)
L. Vega, F. Viñes, K. M. Neyman

How to accurately model IR spectra of silicate granes (poster)
J. Mariñoso, A. Macià, S. T. Bromley

Weak Polyelectrolyte Modelling: Coupling Charge Regulation and Conformational Equilibria vis LEIP Methodology (poster)
J. L. Garcés, P. M. Blanco, S. Madurga, F. Mas

A New Model for Macromolecular Diffusion in Crowded Media: the Chain Entanglement Soft Potential (poster)
P. M. Blanco, S. Madurga, J. L. Garcés, F. Mas

Analysis of the supramolecular structure of helicobacter pyloriurease extracellular at different pHs by molecular dynamics simulation (poster)
H. L. Barazorda-Ccahuana, B. Gómez, F. Mas, S. Madurga

New computational strategies to obtain kinetic data of enzymatic processes in crowded media (poster)
R. Agraso, P. M. Blanco, S. Madurga, F. Mas

Prediction of partition coefficients by ab initio calculations (poster)
L. Saranjan, M. Nedyalkova, V. Simeonov, F. Mas, S. Madurga

Theoretical insight into the active site Dynamics of O-fucosyltransferase 1(poster)
Beatriz Piniello, C. Rovira

Selective hydrogenation from alkynes into alkenes on transition metal carbide surfaces: C_2H_2 activation (poster)
Carlos Andrés Jimenez-Orozco, Elizabeth Florez, Jose Rodríguez

Alzheimer's disease: What can lipophilicity teach us? (poster)
William J. Zamora, J. M. Campanera, K. P. Kepp, F. J. Luque

Framework electron count and estructural trends in [Li_2X_2] rings (poster)
Juan Diego Velasquez, J. Echeverria, S. Alvarez

An introductory workshop in biomedical glycoscience
Donostia (Spain) 3 June 2019

Modeling catalytic mechanisms in carbohydrate-active enzymes (invited talk)
C. Rovira

Delegació del CSIC
Barcelona (Spain) 3 June 2019

La taula periódica com a icona cultural (invited talk)
S. Alvarez

International Meeting on Nanoalloys 2019 (IMN 2019)
Genoa (Italy) 4-7 June 2019

Accuracy of the Topological Approach for nanoalloys: Case study of PtCu nanoparticles (poster)
L. Vega, F. Viñes, K. M. Neyman

Atomic ordering in large bimetallic particles from DFT+Topological calculations (oral communication)
K. M. Neyman

Exploring Complex Free Energy Landscapes: Structure/Function Formation, Multiscales, and Long-timescales
Mainz (Germany) 5 June 2019

How does nature make glycosidic bonds. Insight from enhanced-sampling QM/MM simulations (invited talk)
C. Rovira

Nordic Polymer Days 2019
Trondheim (Norway) 5-7 June 2019

Exploring mechanically-induced charge regulation in weak polyelectrolytes by computer modelling (oral communication)
P. M. Blanco, J. L. Garcés, F. Mas, S. Madurga

XIIth International School on Organometallic Chemistry "Marcial Moreno Mañas"
Castelló de la Plana (Spain) 12-14 June 2019

DFT studies on copper-catalyzed hydroboration/C–C bond formation reactions (oral communication)
J. Jover, E. Ruiz

3rd International Congress of Chemical Engineering (ANQUE-ICCE)
Santander (Spain) 17-18 June 2019

P. Gamallo *(chairman scientific session)*

Molecular modelling applied to post-combustion CO_2 capture and separation (oral communication)
G. Alonso, H. Prats, X. Giménez, F. Llovell, R. Sayós, P. Gamallo

1st Congreso Iberoamericano de Ingeniería Química (CIBIQ)
Santander (Spain) 19-21 June 2019

New materials from computational simulations (oral communication)
S. Kamalinahad, F. Viñes, P. Gamallo

Modelling of phosphonium-based ILs for gas separation from the combination of the soft-SAFT equation of state and COSMO-RS techniques (oral communication)
G. Alonso, P. Gamallo, R. Sayós, F. Llovell

Bioheterocycles 2019. XVIII International Conference on Heterocycles in Biorganic Chemistry
Ghant (Belgium) 20 June 2019

Biradical formation by deprotonation in conjugate 2-amino/imino thiazolew derivatives (poster)
C. Heras, A. San Juan, D. Reta, R. Valero, G. Albareda, N. F. Chilton, A. Fielding, Ibério de P. R. Moreira, J. M. Bofill, F. López-Calahorra

Milestones in Molecular Simulations
London (United Kingdom) 21 June 2019

How carbohydrate-active enzymes work. Insight from enhanced-sampling QM/MM simulations (invited talk)
C. Rovira

5th EUChemS Inorganic Chemistry Conference (EICC-5)
Moscow (Russia) 24-28 June 2019

Computational Modeling of Transition Temperatures in Spin-Crossover Systems (oral communication)
J. Cirera

Computational study of NO single-site disproportionation on Fe^{II}(MOF-5) (oral communication)
J. Jover, C. K. Brozek, M. Dincă, N. López

9è Curs d'Introducció a la Química Computacional (IQTCUB)
Barcelona (Spain) 25-28 June 2019

G. Aullón *(coordinator)*

Universidade Nova de Lisboa
Caparica (Portugal) 26 June 2019

The Periodic Table as a Cultural Icon *(invited talk)*
S. Alvarez

26th Thermodynamics Conference
Punta Umbria (Spain) 26-28 June 2019

Assessing salt-surfactant synergistic effects on interfacial tension from molecular dynamics simulations (oral communication)
G. Alonso, P. Gamallo, A. Mejía, R. Sayós

Interfacial properties of the water + hexane mixture along three-phase line (oral communication)
G. Alonso, M. Cartes, A. Mejía, E. A. Müller

Universidade do Minho
Braga (Portugal) 28 June 2019

Photographers of Chemistry: Art and Documentation (invited talk)
S. Alvarez

20th European Carbohydrate Symposium (EUROCARB)
Leiden (Netherlands) 30 June – 4 July 2019

How carbohydrate-active enzymes work. Insight from computer simulation (plenary conference)
C. Rovira

Oxazoline Or Oxazolinium Ion? The Protonation State and Conformation of the Reaction Intermediate of Chitinase Enzymes (oral communication)
J. Coines, M. Alfonso-Prieto, X. Biarnés, A. Planas, C. Rovira

Catalytic mechanism of β - galactosidases (poster)
A. Nin-Hill, L. Raich, C. Rovira

The Sweet Gateway of Pseudomonads: Sugar Transport Across the OprB Porin (poster)
J. Coines, S. Acosta-Gutiérrez, I. Bodrenko, C. Rovira, M. Ceccarelli

Unveiling the molecular mechanism of a novel oligoxylanase (oral communication and poster)
M. A. B. Morais, J. Coines, M. N. Domingues, R. A. S. Pirolla, C. Rovira, M. T. Murakami

MQM 2019 9th Molecular Quantum Mechanics Conference
Heidelberg (Germany) 5 July 2019

The gentlest ascent dynamics method with conjugate directions: a new and efficient algorithm to locate transition states (poster)
J. M. Bofill, J. Ribas-Ariño, R. Valero, I. de P. R. Moreira, G. Albareda, W. Quapp

Quantum equilibration in a model system porphine (poster)
J. M. Bofill, G. Albareda, I. de P. R. Moreira

Valence tautomerism in organic and organometallic compounds generates unexpected biradical species: a valence bond interpretation (poster)
I. de P. R. Moreira, J. M. Bofill, R. Valero, G. Albareda

The Frenkel-Kontorova Chain (poster)
W. Quapp, J. M. Bofill

19th Meeting of the Spanish Society of Medicinal Chemistry
Vitoria (Spain) 8-11 July 2019

On the bioactive species of azocine-based AChE inhibitors: Interplay between activity and tautomerism (oral communication)
A. Viayna, S. Antermite, C. Altomare, F. J. Luque

XXXVII Reunión bienal Real Sociedad Española de Física
Zaragoza (Spain) 15-19 July 2019

Quantum dynamics of H_2 in SWCNTs: Eigenstates, diffusion and surface coupling (oral communication)
F. Huarte-Larrañaga

CECAM Workshop on Recent developments in quantum dynamics
Lyon (France) 17 July 2019

Approaches to nonadiabatic quantum dynamics without potential-energy surfaces (invited talk)
G. Albareda

35ª Reunió Anual de la XRQTC
Barcelona (Spain) 18 July 2019

Francesc Illas, Silvia Chellini *(co-organization)*

Towards a comprehensive understanding of Pt-based electrocatalysts (invited talk)
Federico Calle-Vallejo

N-Benzyl 4,4-disubstituted piperidines as a potent class of influenza H1N1 virus inhibitors showing a novel mechanism of hemagglutinin fusion peptide interaction (invited talk)
Tiziana Ginex

Vibrational relaxation of diatomic molecules in superfluid helium nanodroplets. Influence of the interaction potential, vibrational energy separation and nanodroplet size (poster)
M. Blancafort, A. Vilà, M. González

A quantum dynamics approach to the rotational relaxation of diatomic molecules inside superfluid helium nanodroplets. Application to some isotope variants of H_2 (poster)
M. Blancafort, A. Vilà, M. González

Unravelling Calmodulin conformational ensemble from combined Molecular Dynamics and FRET simulations (poster)
D. Gonzalo, C. Curutchet

Analysis of the supramolecular structure of helicobacter pyloriurease extracellular at different pHs by molecular dynamics simulation (poster)
H. L. Barazorda-Ccahuana, B. Gómez, F. Mas, S. Madurga

New computational strategies to obtain kinetic data of enzymatic processes in crowded media (poster)
R. Agraso, P. M. Blanco, S. J.L. Garcés, Madurga, F. Mas

Quantum Equilibration in a Model System Porphine (poster)
J. M. Bofill, G. Albareda, I. de P. R. Moreira, R. Valero

Carbon dioxide hydrogenation over the Ni (111) surface: reverse Water-Gas Shift reaction vs Sabatier reaction (poster)
P. Lozano, H. Prats, P. Gamallo, F. Illas, R. Sayós

The 18th International Symposium on Novel Aromatic Compounds (ISNA-18)
Sapporo (Japan) 21 July 2019

Hückel's rule categorizes aromatic closo-boron hydride clústers (oral communication)
J. Poater

Horizon 2020 Project "Materials Networking" Advanced Materials Workshop
Varna (Bulgaria) 21-25 July 2019

Stability or Photoactivity? Porperties of Realistic TiO_2 Nanoparticles (oral communication)
Á. Morales-García, A. Macià, S. T. Bromley, F. Illas

Two Dimensional Transition Metal Carbides/Nitrides (MXenes) as Potential Catalysts for CO_2 Conversion to CO (oral communication)
R. Morales-Salvador, D. Gouveia, Á. Morales-García, F. Viñes, José R. B. Gomes, F. Illas

Correcting Flaws in the Assignment of Nitrogen Chemical Environments in N-doped Graphene (oral communication)
M. Figueras, I. J. Villar-García, F. Viñes, C. Sousa, V. de la Peña O´Shea, F. Illas

First Principles Evaluation of the Initial Oxidation of Transition Metal Surfaces (oral communication)
A. Jurado-Mañas, F. Viñes

Multiscale modeling of spin-crossover phenomena in molecular materials (oral communication)
J. Cirera

XXVI Encontro Nacional de SPQ
Porto (Portugal) 24-26 July 2019

A computational study on the water splitting reaction by MXenes (oral communicationl)
D. Gouveia, Á. Morales-García, F. Viñes, F. Illas, J. R. B. Gomes

XXVIII International Materials Research Congress
Cancun (Mexico) 18-23 August 2019

K. M. Neyman *(co-organization, chairman scientific session)*

Improving accuracy of the topological approach for nanoalloys: Case study of PtCu nanoparticles (poster)
L. Vega, F. Viñes, K. M. Neyman

Accuracy of the topological approach for nanoalloys: Case study of PtCu nanoparticles (poster)
L. Vega, F. Viñes, K. M. Neyman

Metal/metal-oxide interface effects in catalytic nanomaterials: Theory versus experiment (invited talk)
K. M. Neyman

Atomic ordering in large bimetallic particles from DFT+Topological calculations (invited talk)
K. M. Neyman

MCARE 2019
Jeju Island (South Korea) 19-23 August 2019

Designing water splitting catalysts using heuristic rules: advantages, dangers and alternatives (invited talk)
Federico Calle-Vallejo

258th American Chemical Society National Meeting and Exposition
San Diego (USA) 25-29 August 2019

Computational modelling of ceria-based nanocomposite materials for catalysis (invited talk)
K. M. Neyman

Interface effects with oxide supports on the structure and reactivity of metal particles relevant for catalysis (invited talk).
K. M. Neyman

Light & Life - 2019 ESP-IUPB World Congress
(17th International Congress on Photobiology & 18th Congress of the European Society for Photobiology)
Barcelona (Spain) 25-30 August 2019

Multiscale modeling of light harvesting in cryptophyte photosynthesis (oral communication)
C. Curutchet

CECAM/Psi-K School on Density-functional theory and beyond – high-throughput screening and big-data analytics, towards exascale computational materials science
Barcelona (Spain) 26 August – 5 September 2019

E. Ruiz *(organization)*

Hands-on-DFT 2019
Barcelona (Spain) 26 August – 6 September 2019

Unraveling Morphological and Topological Key Aspects of Pd Nanoparticles (poster)
L. Vega, F. Viñes, K. M. Neyman

Subsurface Carbon: A General Feature of Noble Metals (poster)
O. Piqué, I. Z. Koleva, F. Viñes, H. A. Aleksandrov, G. N. Vayssilov, F. Illas

Morphology Dependence of Stability and Properties of Stoichiometric TiO_2 Nanoparticles (poster)
A. Morales-García, A. Macià, S. T. Bromley, F. Illas

CO_2 methanation reaction on the Ni (111) surface: first-principles (poster)
P. Lozano, H. Prats, P. Gamallo, F. Illas, R. Sayós

12th European Conference on Computational and Theoretical Chemistry (EUCO-CTC)
Perugia (Italy) 1-5 September 2019

First-principles-based kinetic Monte Carlo simulations in heterogeneous catalysis:Application to water-gas shift reaction with several catalysts (keynote talk)
R. Sayós, H. Prats, S. Posada-Pérez, J. A. Rodríguez, F. Illas

1st International Conference on Noncovalent Interactions (ICNI2019)
Lisbon (Portugal) 2-6 September 2019

Carbonyl-carbonyl interactions in transition metal complexes (invited talk)
J. Echeverría

Computation and Understanding in Quantum Molecular Science
Toulouse (France), 3-6 September 2019

Continuity and Discontinuity in the Periodic Table (invited talk)
S. Alvarez

8th IAPC Metting
Split (Croatia) 9-11 September 2019

The influence of the background salt in the n-octanol/water distribution coefficient of ionizable drugs (poster)
C. Ràfols, M. Rosés, W. J. Zamora, F. J. Luque

Faraday Discussion: Quantum effects in complex systems
Coventry (United Kingdom) 11-13 September 2019

Kinetic Quantum Sieving of Hydrogen Isotopologues in Carbon Nanotubes: Competition of ZPE effects and Resonance Enhanced Tunneling (poster)
M. Mondelo-Martell, F. Huarte-Larrañaga

7th European Conference on Molecular Magnetism (ECMM 2019)
Florence (Italy) 15-19 September 2019

Magnetism and electronic transport in Bisdithiazolyl-based multifunctional materials: a computational study (poster)
C. Roncero

Revising the common understanding of metamagnetism in the molecule-based bisdithiazolyl BDTMe compound (poster)
M. Deumal

Encapsulating Mononuclear Single Molecule Magnets (oral communication)
S. Gómez-Coca, M. Amoza, L. Maxwell, E. Ruiz

European Materials Research Symposium Fall Meeting 2019 – Symposium Q
Varsaw (Poland) 16 September 2019

Breaking scaling relations does not always lead to enhanced OER electrocatalysts (invited talk)
Federico Calle-Vallejo

Tracking the Properties of Oxides from Nanoparticle to Bulk (oral communication)
S. T. Bromley

Understanding the Interplay between Size, Morphology and Energy Gap in Photoactive TiO_2 Nanoparticles (oral communication)
S. T. Bromley

Interplay between Size, Morphology and Energy Gap in Realistic TiO_2 Nanoparticles (oral communication)
Á. Morales-García, A. Macià, S. T. Bromley, F. Illas

The 23rd International conference on "Horizons in Hydrogen Bond Research" (HBOND2019)
Amsterdam (Netherlands) 23 September 2019

Non-terran biosolvents model structure, stability and replication of B-DNA (invited talk)
J. Poater, T.A. Hamlin, C. Fonseca Guerra, F.M. Bickelhaupt

XI International Conference on Mechanisms of Catalytic Reactions
Sochi (Russia) 7 – 11 October 2019

K. M. Neyman *(scientific committee and chaiman scientific session)*

Metal/metal-oxide interface effects in catalytic materials: Theory versus experiment (oral communication)
K. M. Neyman

Blas Cabrera 2019 Physics Seminar
Tenerife (Spain) 16 October 2019

Tailoring Low-Dimensional Materials with Impact on the Activation of CO_2 and on Photocatalysis (invited talk)
Á. Morales-García

22nd Conference on Process Integration for Energy Saving and Pollution Reduction - PRES'19
Creta (Greece) 20-23 October 2019

Integrated Reaction-Separation Processes Sequencing and Screening at Early Stages of Design (invited talk)
K. Marin, J. Bonet-Ruiz, A. E. Plesu Popescu, V. Plesu, P. Iancu, J. Llorens

Hydration of Cyclohexene to Cyclohexanol In A Hybrid Reactive Distillation with A Side Decanter (poster)
I. Marchante, A. E. Plesu Popescu, V. Plesu, J. Bonet-Ruiz, P. Iancu, J. Llorens

Energy Consumption in Sharp and Non-Sharp Splits of Ideal Ternary Mixtures (poster)
S. Exposito, V. Plesu, J. Bonet-Ruiz, A. E. Plesu Popescu, P. Iancu, J. Llorens

Symposium "Advances in cluster beam deposition"
Okinawa (Japan) 20-25 November 2019

Metal/metal-oxide interface effects in catalytic nanomaterials: Theory versus experiment (oral communication)
K. M. Neyman

The 3rd Sustainable Process Integration Laboratory Scientific Conference: Energy, Water, Emission & Waste in Industry and Cities
Brno (Czech Republic) 21-22 November 2019

Bioethanol dehydration process in a gasoline-mixing process (poster)
J. L. Pellín, A.E. Plesu, J. Bonet, J. Llorens

Concentration of orthophosphate and ammonium via forward osmosis to precipitate them as struvite (poster)
J. Labanda, J. Llorens, A. E. Plesu, J. Bonet

SancaMedChem2019 - The Sao Carlos Special Medicinal Chemistry Meeting
Sao Carlos (Brasil) 25-27 November 2019

Disclosing the molecular determinants of bioactive compounds: From chemical structure to mechanisms of drug action (oral communication)
F. J. Luque

Advances in Computational Biology (AdvCompBio 2019)
Barcelona (Spain) 28-29 November 2019

Model-driven discovery of metabolic reprogramming associated to metastatic cancer and cisplatin resistance (poster)
M. Cascante, C. Balcells, C. Foguet, M. Tarrado, O. Camacho, P. de Atauri, T. Thomson, F. Mas, S. Marin

Scientific Advisory Board Meeting of the IQTC-UB
Barcelona (Spain) 29 November 2019

Unravelling Calmodulin conformational ensemble from combined Molecular Dynamics and FRET simulations (poster)
D. Gonzalo, C. Curutchet

Dual classical/quantum MD strategy for the determination of site energies in photosynthetic complexes: Application to the PC645 antenna (poster)
B. Ozaydin, M. Corbella, C. Curutchet

First-Principles Evaluation of the Initial Oxidation of Transition Metal Surfaces (poster)
A. Jurado-Mañas, F. Viñes, F. Illas

Morphology Dependence of Stability and Properties of Stoichiometric TiO_2 Nanoparticles (poster)
Á. Morales-García, A. Macià, S. T. Bromley, F. Illas

H_2 Dissociation on Transition Metal Carbide Surfaces (poster)
J. J. Piñero, P. J. Ramírez, S. T. Bromley, F. Illas, F. Viñes, J. A. Rodríguez

Unraveling Morphological and Topological Key Aspects of Pd Nanoparticles (poster)
L. Vega, F. Viñes, K. M. Neyman

Accuracy of the Topological Approach for Nanoalloys: Case Study of PtCu Nanoparticles (poster)
L. Vega, F. Viñes, K. M. Neyman

X-Ray Photoelectron Spectroscopy: Theoretical Approach (poster)
M. Figueras, I. J. V. García, F. Viñes, C. Sousa, V. A. de la Peña O'Shea, F. Illas

Tuning Activity of Transition Metal Carbides by Surface Metal Alloying: Case of Study of CO_2 Capture (poster)
M. López, L. Broderick, J. Carey, F. Viñes, M. Nolan, F. Illas

Subsurface Carbon: A General Feature of Noble Metals (poster)
O. Piqué, I. Z. Koleva, F. Viñes, H. A. Aleksandrov, G. N. Vayssilov, F. Illas

Grazynes: A New Family of Carbon-Based Materials from IQTCUB (poster)
P. Gamallo, F. Viñes

CO_2 Methanation Reaction on the Ni(111) Surface: First-Principles Kinetic Monte Carlo Study (poster)
P. Lozano, H. Prats, P. Gamallo, F. Illas, R. Sayós

Weak Polyelectrolyte Modelling: Coupling Charge Regulation and Conformational Equilibria vis LEIP Methodology (poster)
J. L. Garcés, P. M. Blanco, S. Madurga, F. Mas

A New Model for Macromolecular Diffusion in Crowded Media: the Chain Entanglement Soft Potential (poster)
P. M. Blanco, S. Madurga, J. L. Garcés, F. Mas

Effect of pH on conformational behaviour in peptides. Simulation of polyaspartic acid (poster)
C. Privat, S. Madurga, F. Mas, J. Rubio.

Analysis of the supramolecular structure of helicobacter pyloriurease extracellular at different pHs by molecular dynamics simulation (poster)
H. L. Barazorda-Ccahuana, B. Gómez, F. Mas, S. Madurga

Prediction of partition coefficients by ab initio calculations (poster)
L. Saranjan, M. Nedyalkova, V. Simeonov, F. Mas, S. Madurga

3rd International Caparica Christmas Conference on Translational Chemistry 2019
Lisbon (Portugal) 2 December 2019

Open-shell Jellium aromaticity in metal clústers (invited talk)
J. Poater, M. Solà

3rd International Caparica Christmas Conference on Translational Chemistry (IC3TC)
Caparica (Portugal) 2-5 December 2019

Molecular Magnetism: Tailoring Mononuclear Single Molecule Magnets behaviour of First-Row Transition Metal Complexes (comunicació oral)
S. Gómez-Coca, E. Ruiz

RESEARCH STAYS IN RECOGNIZED CENTERS

Alemany, P.	**Universidad Católica del Norte (Chile)** UB visiting researcher invited by Jaime Llanos. May 2019
Alemany, P.	**Donostia International Physics Center, Donostia (Spain)** UB visiting researcher invited by Abel Carreras. December 2019
Bernuz, E.	**Donostia International Physics Center, Donostia (Spain)** UB visiting researcher invited by Abel Carreras. December 2019
Curutchet, C.	**Universitat Federal d'ABC, Santo André (Brasil)** Research stay with Prof. Paula Homem-de-Mello. September 2019
Ginex, T.	**University of Bristol, Bristol (United Kingdom)** Research stay with Prof. Adrian Mulholland. February 2019
López Berbel, M.	**Tyndall National Institut, Cork (Ireland)** Research stay with Prof. Michael Nolan. June-August 2019
Llunell, M.	**Donostia International Physics Center, Donostia (Spain)** UB visiting researcher invited by Abel Carreras. December 2019
Neyman, K. M.	**University of Sofia, Sofia (Bulgaria)** Invited visiting researcher. May 2019
Nin-Hill, A.	**University of York, York (United Kingdom)** Research stay with Prof. Gideon J. Davies. April-June 2019
Rovira, C.	**University of York, York (United Kingdom)** Research stay with Prof. Gideon J. Davies. May-October 2019

PARTICIPATION IN COMPETITIVE FUNDED RESEARCH PROJECTS

Institute of Theoretical and Computational Chemistry, (Excelence Unit "María de Maeztu").
E. Ruiz, University of Barcelona
MdM-2017-0767, 2018-2021
Ministry of Economy and Competitiveness (MINECO)
Amount: 2.000.000 EUR

Estructura Electrónica y Propiedades en Moléculas y Sólidos Inorgánicos.
E. Ruiz, University of Barcelona
PGC2018-093863-B-C21, 2019-2021
Ministry of Economy and Competitiveness (MINECO)
Amount: 210.000 EUR

Estructura electrónica y propiedades de moléculas y sólidos inorgánicos.
P. Alemany, K. Neyman, University of Barcelona
PGC2018-093863-B-C22, 2019 – 2021
Ministry of Economy and Competitiveness (MINECO)
Amount: 121.000€

Diseño Racional de Nuevos Catalizadores Heterogeneos, Electrocatalizadores y Fotocatalizadores Para la Produccion de Energia Limpia Sostenible a Traves de la Conversion de H_2.
F. Illas, University of Barcelona
RTI2018-095460-B-I00/AEI/FEDER, 2019 – 2021
Ministry of Economy and Competitiveness (MINECO)
Amount: 229.900 EUR

Química Computacional Aplicada para la captura, separación y conversión de CO_2 en combustibles ligeros.
R. Sayós, P. Gamallo, University of Barcelona
RTI2018-094757-B-I00/AEI/FEDER, 2019 – 2021
Ministry of Economy and Competitiveness (MINECO)
Amount: 85.426 EUR

Modeling and Simulation of reactive processes in enzymes by means of ab initio molecular dynamics and QM/MM methods.
C. Rovira, University of Barcelona
CTQ2017-85496-P/AEI/FEDER, 2018-2020
Ministry of Economy and Competitiveness (MINECO)

Diseño racional desde una perspectiva computacional de materiales basados en radicales orgánicos con propiedades de interés tecnológico.
M. Deumal, J. J. Novoa, University of Barcelona
CTQ2017-87773-P/AEI/FEDER, 2018-2020
Ministry of Economy and Competitiveness (MINECO)

Structure-based modeling of the role of the environment in photosynthetic light harvesting and protein fluorescence.
C. Curutchet, University of Barcelona
CTQ2017-89924-P/AEI/FEDER, 2018-2020
Ministry of Economy and Competitiveness (MINECO)
Amount: 65.340 EUR

Estudio Computacional del Control Mecanoquímico de Reacciones de Interés en Química Biorgánica.
J. M. Bofill, I. de P. R. Moreira, University of Barcelona
CTQ2016-76423-P/AEI/FEDER, 2017-2019
Ministry of Economy and Competitiveness (MINECO)
Amount: 36.300 EUR

Diseño computacional de pares de bases de ADN artificiales que pueden ser replicados.
J. Poater, University of Barcelona
CTQ2016-77558-R/AEI/FEDER, 2016-2019
Ministry of Economy and Competitiveness (MINECO)

Producción de bio-plásticos a partir de la fracción orgánica de residuos municipales.
J. Mata, J. Llorens, University of Barcelona
CTM2016-76275-R, 2016-2020
Ministry of Economy and Competitiveness (MINECO)
Amount: 139.150 EUR

Understanding, controlling and optimizing heterogeneous catalysts and photocatalysts at the nanoscale. Application to carbon dioxide conversion and hydrogen production.
F. Illas, S. T. Bromley, University of Barcelona
CTQ2015-64618-R/AEI/FEDER, 2016-2019
Ministry of Economy and Competitiveness (MINECO)

Computational Materials Science Laboratory.
F. Illas, University of Barcelona
2017 SGR 13, 2018-2021
University and Research Grants Management Agency (AGAUR)
Amount: 68.000 EUR

Modelització i Disseny de Sistemes Químics Radicalaris.
J. M. Bofill, University of Barcelona
2017 SGR 348, 2018-2020
University and Research Grants Management Agency (AGAUR)
Amount: 20.000 EUR

Grup de Bioinformàtica Integrativa.
M. Cascante, University of Barcelona
2017 SGR 1033, 2017-2020
University and Research Grants Management Agency (AGAUR)

Grup de recerca consolidat: Estructura i funció en macromolècules.
C. Rovira, University of Barcelona
2017 SGR 1189, 2017-2020
University and Research Grants Management Agency (AGAUR)

Grup d'Estructura Electrònica.
S. Alvarez, University of Barcelona
2017 SGR 1289, 2017-2019
University and Research Grants Management Agency (AGAUR)
Amount: 44.480 EUR

Biologia Computacional i Disseny de Fàrmacs.
F. J. Luque, University of Barcelona
2017 SGR 1746, 2017-2020
University and Research Grants Management Agency (AGAUR)

Theoretical study on the receptor-cannabinoid affinities and dynamics.
C. Curutchet, University of Barcelona
2018 DI 043, 2019-2021
Catalan Government (GENCAT)
Amount: 21.600 EUR

Beca Postdoctoral Beatriu de Pinós.
Silvia Gómez-Coca, University of Barcelona
2017 BP 00080, 2018-2020
Catalan Government (GENCAT)
Amount: 90.000 EUR

Captura de CO_2 emitido por vehiculo basados en motores de combustión, mediante absorció en sólidos porosos.
X. Gimenez, P. Gamallo, University of Barcelona
IDI-20190124, 2019-2021
Center for Industrial Technological Development (CDTI), Recam Laser S.L.
Amount:146.000 EUR

Deciphering the Metabolism of Haematological Cancers (HaemMetabolome).
M. Cascante, University of Barcelona
8P1MCA - H2020. PILLAR 1-EXCELLENT SCIENCE. MCA. Marie Sklodowska-Curie Actions, **675790**, 2015-2019
European Union

Tuning Tubulin Dynamics and Interactions to Face Neurotoxicity: a Multidisciplinary Approach for Training and Research (TubInTrain).
M. Cascante, University of Barcelona
860070 – H2020-MSCA-ITN-2019, 2019- 2023
European Union

Instituto Nacional de Bioinformática.
M. Cascante, University of Barcelona
Ayudas para proyectos de investigación del área de Ciencias de la Salud (FIS), 2018-2020
Ministry of Economy and Competitiveness (MINECO)

Training interdisciplinary glycoscientists to get a molecular-level grip on glycocodes at the human mucosa–microbiota interface.
C. Rovira, University of Barcelona
814102-SWEET CROSSTALK, 2019-2022
European H2020 Programme

Recuperació i valorilzació de recursos de digestats urbans en el marc de l'economía circular (DIGESTAKE).
J. F. Garcia, University of Barcelona
COMRDI16-1-0061-01, 2017 – 2020
Acció, Catalan Business Suport Agency
Amount: 117.934 EUR

Energy and charge transfer by non-orthogonal configuration interaction
C. Sousa, M. Llunell, University of Barcelona
CHM154, 2019-2020
Oak Ridge Leadership Computing Facility (USA)

Mecanismos moleculares implicados en la inhibición de dianas para tratamientos anti-influenza: canal de protones M2 y hemaglutinina.
F. J. Luque, University of Barcelona
SAF-2017-88107-R, 2018-2020
Ministry of Economy and Competitiveness (MINECO)
Amount: 90.750 EUR

Identificación, síntesis y evaluación toxicológica de molécula propia antidetonante.
F. J. Luque, University of Barcelona
FBG-309799, 2018-2019
REPSOL-YPF, SA
Amount: 98.780 EUR

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).
K. Neyman, University of Barcelona
8SEWP - H2020. SEWP. Spreading Excellence and Widening Participation, 2016-2019
European Union

QUIFIEXP - Química Física Experimental.
J. Ignes, University of Barcelona
GINDO-UB/112, 2016-2019
PPID – Teaching Innovation Projects (UB)

ICREA Acadèmia.
F. Illas, University of Barcelona
2016-2020
Catalan Institute for Advanced Research (ICREA, Generalitat de Catalunya)

Synthesis and characterization of the structural modifications of Y_2WO_6:RE /TiO_2 core/shell nanoparticles (RE^{3+} = Eu, Sm and Gd, Er and the couple Er/Yb) and their use as photoelectrodes for the improvement of the efficiency of red and NIR sunlight harvesting in DSSCs.
J. Llanos, North Catholic University, Antofagasta (Chile), P. Alemany, University of Barcelona
Fondecyt, 1181302, 2018-2021
CONICYT

COST Action CA18234 – Computational materials sciences for efficient water splitting with nanocrystals from abundant elements
M. Caspary Toroker, TECHNION, Haifa, Israel
European Commission, 2019-2023
European Cooperation in Science and Technology Program

Estudi de laboratori i planta pilot per la recuperació d'amoni dels purins.
J. Mata Álvarez, F. Mas, University of Barcelona
Private company contract, 2017-2019
INDUKERN (Veterinary division)

Reactivity of lattice oxygen in nanostructured CeO_2 doped by Pt and Pd.
K. Neyman, University of Barcelona
QCM-2018-3-0018, 2018-2019
Spanish Supercomputing Network (RES)

Atomic ordering in bimetallic nanoparticles of fcc-type: Pt-Ni.
K. Neyman, University of Barcelona
QCM-2019-1-0032, QS-2019-2-0022, 2019
Spanish Supercomputing Network (RES)

Striking chemical orderings in bimetallic nanoparticles with silver and gold atomic shells.
K. Neyman, University of Barcelona
QS-2019-3-0023, 2019-2020
Spanish Supercomputing Network (RES)

Institut de Química Teòrica i Computacional