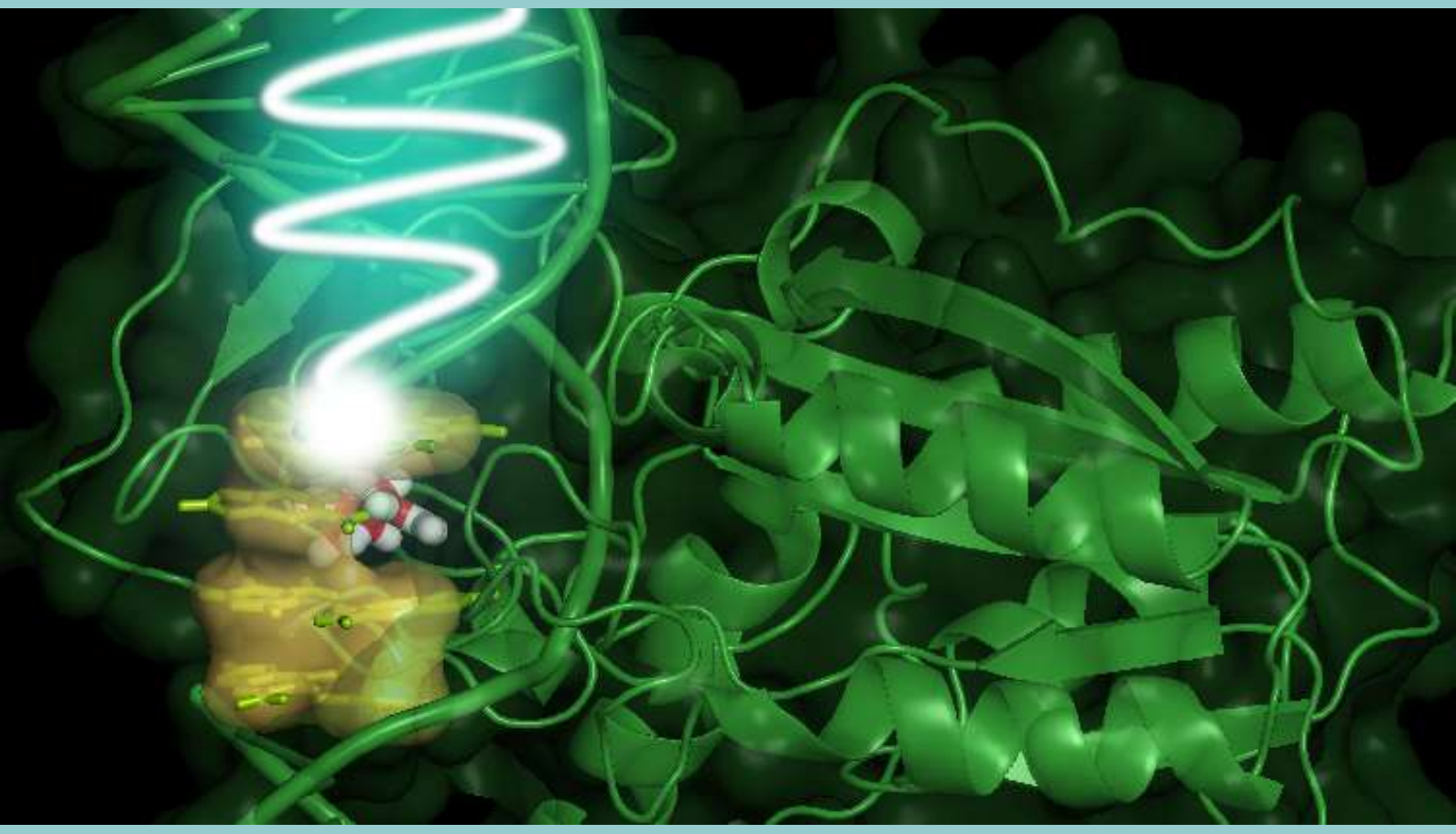
Institut de Química Teòrica i Computacional

EXCELENCIA MARÍA DE MAEZTU

UNIVERSITAT DE BARCELONA

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

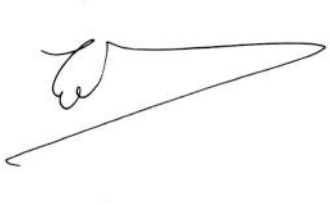


Activity Report 2020

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. 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 past year has been a complicated one for all of humanity. In spite of this fact, it is worth mentioning the effort made by the researchers of our Institute to maintain research at a level equivalent to, or even higher than, previous years as it is reflected in this memory.

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 IQTCUB'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

REPORT CONTENT

I. IQTCUB OVERVIEW

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

I.1 DIRECTION TEAM

The IQTCUB direction team during 2020 has been,

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

Other Categories (Professors Agregats)

Bonet Ruiz	Jordi	SPAIN (M)	Chem. Engineering & Analytical Chem.
Gamallo Belmonte	Pablo	SPAIN (M)	Materials Science & Physical Chemistry
Madurga Díez	Sergio	SPAIN (M)	Materials Science & Physical Chemistry
Reigada Sanz	Ramón	SPAIN (M)	Materials Science & Physical Chemistry
Ribas Ariño	Jordi	SPAIN (M)	Materials Science & Physical Chemistry
Viñes Solana	Francesc	SPAIN (M)	Materials Science & Physical Chemistry

ICREA Research Professors

Bromley	Stefan T.	UK (M)	Materials Science & Physical Chemistry
Neyman	Konstantin	GERMANY (M)	Materials Science & Physical Chemistry
Poater Teixidor	Jordi	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
Puigmartí-Luis	Josep	SPAIN (M)	Materials Science & Physical Chemistry
Rovira Virgili	Carme	SPAIN (F)	Inorganic Chemistry & Organic Chemistry

Other Categories (Professors Lectors)

Bidon-Chanal Badia	Axel	SPAIN (M)	Nutrition, Food Sciences & Gastronomy
Jover Modrego	Jesús	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
Plesu Popescu	Alexandra El.	SPAIN (F)	Chem. Engineering & Analytical Chem.

Other Categories (Professors Associats)

Cremades Martí	Eduard	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
Jurado Mañas	Anabel	SPAIN (F)	Materials Science & Physical Chemistry
López Marne	Estefanía	SPAIN (F)	Materials Science & Physical Chemistry
Vázquez Lozano	Javier	SPAIN (M)	Nutrition, Food Sciences & Gastronomy
Viayna Gaza	Antonio	SPAIN (M)	Nutrition, Food Sciences & Gastronomy

Postdoctoral contracts

Beatriu de Pinós-Juan de la Cierva

Bruix Fusté	Albert	SPAIN (M)	Materials Science & Physical Chemistry
Gómez Coca	Silvia	SPAIN (F)	Inorganic Chemistry & Organic Chemistry
Liao	Quinhua	CHINA (M)	Inorganic Chemistry & Organic Chemistry
Llabrés Prats	Salomé	SPAIN (F)	Nutrition, Food Sciences & Gastronomy
Morales García	Ángel	SPAIN (M)	Materials Science & Physical Chemistry

Ramón y Cajal

Calle Vallejo	Federico	COLOMBIA (M)	Materials Science & Physical Chemistry
Cirera Fernández	Jordi	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
Echeverría López	Jorge	SPAIN (M)	Inorganic Chemistry & Organic Chemistry

Contracte Projecte de Recerca

Alonso Benito	Gerard	SPAIN (M)	Materials Science & Physical Chemistry
Belce	Yonca	TURKEY (F)	Materials Science & Physical Chemistry
Escartín Esteban	José María	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
Ginex	Tiziana	SPAIN (F)	Nutrition, Food Sciences & Gastronomy
Mattera	Michele	ITALY (M)	Materials Science & Physical Chemistry
Prats García	Hèctor	SPAIN (M)	Materials Science & Physical Chemistry
Rodríguez San Miguel	David	SPAIN (M)	Materials Science & Physical Chemistry
Sorrenti	Alessandro	ITALY (M)	Materials Science & Physical Chemistry
Sun	Xiaobo	CHINA (M)	Inorganic Chemistry & Organic Chemistry

Other

Albareda Piquer	Guillem	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
Kolb	Manuel	GERMANY (M)	Materials Science & Physical Chemistry
Valero Montero	Rosendo	SPAIN (M)	Materials Science & Physical Chemistry
Vilà Casanovas	Arnau	SPAIN (M)	Materials Science & Physical Chemistry

Ph.D. Students

Beca Programa María de Maeztu

Colomer Llombart	Eduard	SPAIN (M)	Materials Science & Physical Chemistry
Lleopart Motis	Genis	SPAIN (M)	Materials Science & Physical Chemistry
Morales Salvador	Raúl	SPAIN (M)	Materials Science & Physical Chemistry
Privat Contreras	Cristian	SPAIN (M)	Materials Science & Physical Chemistry
Vidal Ramon	Daniel	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
Vílchez Pérez	David	SPAIN (M)	Nutrition, Food Sciences & Gastronomy

FI Grant (Catalan Government Program)

Aledavood	Elnaz	SPAIN (F)	Nutrition, Food Sciences & Gastronomy
Blanco Andrés	Pablo Miguel	SPAIN (M)	Materials Science & Physical Chemistry
Macià Escatllar	Antoni	SPAIN (M)	Materials Science & Physical Chemistry
Mariñoso Guiu	Joan	SPAIN (M)	Materials Science & Physical Chemistry
Martín Rodríguez	Alejandro	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
Nin Hill	Alba	SPAIN (F)	Inorganic Chemistry & Organic Chemistry
Piniello Castillo	Beatriz	SPAIN (F)	Inorganic Chemistry & Organic Chemistry
Vega Domínguez	Lorena	SPAIN (F)	Materials Science & Physical Chemistry

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

Almacellas Salillas	David	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
Bernuz Fitó	Efrem	SPAIN (M)	Materials Science & Physical Chemistry
Cánovas Montes	Manuel Ant.	SPAIN (M)	Materials Science & Physical Chemistry
Cuxart Sánchez	Irene	SPAIN (F)	Inorganic Chemistry & Organic Chemistry
Esquivias Baut. Lisb.	Oriol	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
Gómez Mudarra	Francisco A.	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
Piñero Vargas	Juan José	SPAIN (M)	Materials Science & Physical Chemistry
Piqué Caufapé	Oriol	SPAIN (M)	Materials Science & Physical Chemistry
Recio Poo	Miguel	SPAIN (M)	Materials Science & Physical Chemistry
Regalado Aguilar	Mauricio	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
Santiago Piera	Raúl	SPAIN (M)	Materials Science & Physical Chemistry

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

Lozano Reis	Pablo	SPAIN (M)	Materials Science & Physical Chemistry
Vila Julià	Guillem	SPAIN (M)	Materials Science & Physical Chemistry
Vilaplana Saiz	Marta	SPAIN (F)	Materials Science & Physical Chemistry

ITN UE Grant

Mnevets	Daniil	BELARUS (M)	Inorganic Chemistry & Organic Chemistry

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

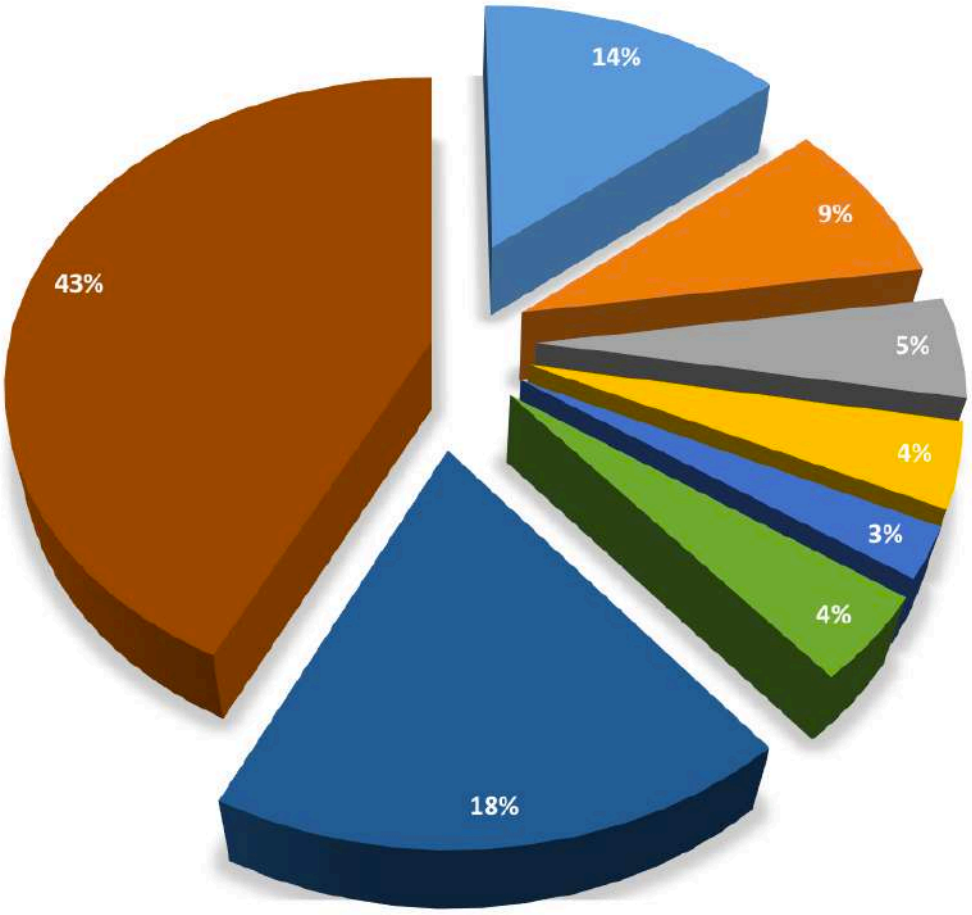
López Berbel	Martí	SPAIN (M)	Materials Science & Physical Chemistry
Gonzalo Palao	Daniel	SPAIN (M)	Pharm. & Pharm. Tech. & Phys. Chem.
Navarro Maestro	Laia	SPAIN (F)	Inorganic Chemistry & Organic Chemistry
Roncero Barrero	Cristina	SPAIN (F)	Materials Science & Physical Chemistry
Svobodova	Adela	SPAIN (F)	Materials Science & Physical Chemistry
Velásquez Benites	Juan Diego	SPAIN (M)	Inorganic Chemistry & Organic Chemistry

Beca Doctorat Industrial

Espel Grekopoulos	Joan	SPAIN (M)	Pharm. & Pharm. Tech. & Phys. Chem.

Other

Barazorda-Ccahuana	Haruna	PERU (F)	Materials Science & Physical Chemistry
Campos-Vicens	Lluís	SPAIN (M)	Nutrition, Food Sciences & Gastronomy
Coines López-Nieto	Joan	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
Figueras Valls	Marc	SPAIN (M)	Materials Science & Physical Chemistry
García Gonzalo	Lluc	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
Kamalinahad	Saedeh	IRAN (F)	Materials Science & Physical Chemistry
Morales Salvador	Raúl	SPAIN (M)	Materials Science & Physical Chemistry
Nicholas	James	UK (M)	Materials Science & Physical Chemistry
Ozaydin	Gül Beste	TURKEY (F)	Pharm. & Pharm. Tech. & Phys. Chem.
Saranjam	Leila	IRAN (F)	Materials Science & Physical Chemistry
Tarik	Karim	SPAIN (M)	Materials Science & Physical Chemistry
Valdivia	Aitor	SPAIN (M)	Nutrition, Food Sciences & Gastronomy
Velasco	Arnau	SPAIN (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, technical staff members take care of maintenance of the computational infrastructure and give support to the research groups. Their work is extremely important since they also implement the codes and optimize their performance.

Jordi Inglés Camats	*HPC System Administrator Manager*
Irene Zamora Carretero	*HPC System Administrator*
Silvia Chellini	*Research Support Team*
Begoña López Maestre	*Research Support Team*
Patricia Verdugo Salomón	*3D Designer*

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	22 nodes
Notes	64 bits processors

Specifications

22 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)

iqtc09 (*invested value 297.000 €*)

Machine type	Gigabyte Cluster
Operating System	Centos 7.2
Services	Calculation cluster
Structure	26 nodes
Notes	64 bits processors

Specifications

26 Gigabyte R13
CPU: 2 x 2,9 GHz AMD EPYC 7542 32-core
RAM: 1 TB
HD: 1 x 2 TB SATA hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (internal data network)
Network: 2 x 10gigabit network card

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

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 4.500 €*)
Machine type Portal access servers
Operating system Debian stable/ Debian 10.5
Services SGE Execution Host, Heartbeat, ssh server
Structure 3 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) + 1 IPMI card (OOB)

1 DELL Poweredge R640 node
CPU: 1 x 2,2 GHz Xeon Silver 4210
RAM: 16 GB
HD: 1 x 256 GB hard disk
Network: 2 gigabit network card (internal network) + 1 IPMI card (OOB)

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 144TB of space, ~3TB/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. 2 MSI LAPTOP with Oculus RIFT S -Virtual Reality Study-.
14. 1 XYZ printing da Vinci Color AIO 3D printer.
15. 3 Oculus Quest.

The approximated invested cost of this equipment is *56.000 €.*

SUMMARY

Cores.....5,726 c

Memory ..... 64,886 GB RAM

Calculation disk capacity.....318 TB

Data user disk capacity.....80 TB

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

*2.410.000 €**

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

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

II. IQTCUB ACTIVITIES

II.1 GENERAL ACTIVITIES

Next, a description of activities and actions promoted by IQTCUB through 2020 is provided.

a. ***Promotion and encouragement of research.*** This year the IQTCUB has offered two Master's degree grant and three Post-Master grants aimed to help students to initiate a scientific career. These grants are addressed to students about to end the degree or master for collaborating in some of the research projects of the IQTCUB groups. The MSc grants have been awarded to Eloi Sánchez Ambrós and Néstor Mauricio García-Romeral and the Post-Master ones to Ling Meng, Gul Beste Ozaydin and Riccardo Farris. More information at https://www.iqtc.ub.edu/education-outreach/fellowships/

Total cost: 2.000 € (MSc grant) and 3.000 € (Post-MSc grant)

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

b. ***Women in the Scientific Research.*** This one-day workshop aimed at the dissemination of the research done by scientific women. It took place on February 11th, 2020. Among the participants PhD. Roberta Sinatra from University of Copenhagen, PhD. Joaquina Álvarez from CSIC and PhD. Núria Salan from UPC.

Panel of the workshop.

c. ***Scientific Dissemination Activities.*** Prof. Xavier Giménez Font has been involved in the following scientific and teaching dissemination activities during 2020:

1. "Més petit i millor impossible: les promeses dels motors moleculars". Toc–Toc UB Science Dissemination Program, Institut de Vilafant, Vilafant, 8/Jan/2020.
2. "UB s'Apropa 20". Institut Manuel Blancafort, La Garriga, 9/Jan/2020.
3. "UB s'Apropa 20". Col·legi Pare Manyanet, Barcelona, 14/Jan/2020.
4. "L'Aire que Respirem", Toc–Toc UB Science Dissemination Program, Agrupació Astronòmica de Sabadell, Sabadell. 15/Jan/2020.
5. "UB s'Apropa 20". Institut Creu de Saba, Olesa de Montserrat, 16/Jan/2020.
6. "UB s'Apropa 20". Institut Joan Brossa, Barcelona, 16/Jan/2020.
7. "UB s'Apropa 20". Institut Montserrat Miró, Montcada i Reixac, Social & Human Science students, 17/Jan/2020.
8. "UB s'Apropa 20". Institut Montserrat Miró, Montcada i Reixac, Experimental Science & Technology students, 17/Jan/2020.
9. "L'Aire que Respirem", Toc–Toc UB Science Dissemination Program, Institut Maria Espinalt, Barcelona. 17/Jan/2020.
10. "UB s'Apropa 20". Institut Angeleta Ferrer i Sensat, Sant Cugat del Vallès, Group A students, 20/Jan/2020.
11. "UB s'Apropa 20". Institut Angeleta Ferrer i Sensat, Sant Cugat del Vallès, Group B students, 20/Jan/2020.
12. "UB s'Apropa 20". Institut Vil·la Romana, La Garriga, 21/Jan/2020.
13. "UB s'Apropa 20". Institut Joan Oliver, Sabadell, 22/Jan/2020.
14. "UB s'Apropa 20". Institut de Mollet, Mollet del Vallès, 23/Jan/2020.
15. "UB s'Apropa 20". Institut El Cairat, Esparreguera, 23/Jan/2020.
16. "UB s'Apropa 20". Institut Montserrat Colomer, Sant Esteve Sesrovires, 24/Jan/2020.
17. "UB s'Apropa 20". Saint Nicholas School, Barcelona, 24/Jan/2020.
18. "UB s'Apropa 20". Institut Pau Vila, Sabadell, 29/Jan/2020.
19. "UB s'Apropa 20". Institut Lauro, Les Franqueses del Vallès, 30/Jan/2020.
20. "UB s'Apropa 20". Institut Vinyet, Sitges, 31/Jan/2020.
21. "UB s'Apropa 20". Institut Jaume Balmes, Barcelona, 31/Jan/2020.
22. "UB s'Apropa 20". Institut Lluís de Requesens, Molins de Rei, 3/Feb/2020.

23. “UB s’Apropa 20”. Institut Miramar, Viladecans, 4/Feb/2020.
24. “UB s’Apropa 20”. Escola Jesuïtes Sant Gervasi — Infant Jesús, Barcelona, 6/Feb/2020.
25. “UB s’Apropa 20”. Institut Joaquima Pla i Farrera, Sant Cugat del Vallès, 7/Feb/2020.
26. “UB s’Apropa 20”. Institut Polinyà, Polinyà, 7/Feb/2020.
27. “UB s’Apropa 20”. Institut La Roca, La Roca del Vallès, 13/Feb/2020.
28. “UB s’Apropa 20”. Escola Montagut, Vilafranca del Penedès, 13/Feb/2020.
29. “L’origen dels elements químics”. Toc–Toc UB Science Dissemination Program, Institut Salvador Dalí, El Prat de Llobregat, 14/Feb/2020.
30. “UB s’Apropa 20”. Institut Vescomtat Cabrera, Hostalric, 17/Feb/2020.
31. “UB s’Apropa 20”. Institut Sentmenat, Sentmenat, 19/Feb/2020.
32. “UB s’Apropa 20”. Institut Miramar, Viladecans, 20/Feb/2020.
33. “UB s’Apropa 20”. Institut Torre de Malla, Parets del Vallès, 26/Feb/2020.
34. “UB s’Apropa 20”. Institut Creu de Saba, Olesa de Montserrat, 27/Feb/2020.
35. “UB s’Apropa 20”. Institut Les Termes, Sabadell, 27/Feb/2020.
36. “UB s’Apropa 20”. Escola Pia, Caldes de Montbui, 2/Mar/2020.
37. “UB s’Apropa 20”. Escola Daina Isard, Olesa de Montserrat, 4/Mar/2020.
38. “UB s’Apropa 20”. Institut Voltreganès, Les Masies de Voltregà, 5/Mar/2020.
39. “Apropa’t a la UB 20”. Talk for Escola Lleó XIII, Universitat de Barcelona, 6/Mar/2020.
40. “Metales tóxicos, y sus efectos ambientales y sobre la salud humana”, On–line Seminar, Biological Inorganic Chemistry course, Universidad de Sevilla, 29/April/2020.
41. “Llibres de Divulgació Científica”, Màster de Comunicació Especialitzada, Univ. Barcelona, 9/Nov/2020.
42. “La Màgia de l’Aigua”. Toc–Toc UB Science Dissemination Program, Institut Escola Eixample, Barcelona, 16/Nov/2020.
43. “La Màgia de l’Aigua”. Toc–Toc UB Science Dissemination Program, Institut Escola Eixample, Barcelona, 19/Nov/2020.

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

1. "Óxido de etileno: qué es, para qué se usa, y que efectos tiene para tu salud si lo respiras". Interview by José Pichel, El Confidencial Journal, January 14th, 2020: https://www.elconfidencial.com/tecnologia/ciencia/2020-01-15/explosion-tarragona-causas-problemas-efectos_2412020/

2. "Què és l'òxid d'etilè? Per què és tan inflamable?". Interview by Pere Renom and Helena Garcia Melero, program "Tot es mou", TV3. January 15th, 2020: https://www.ccma.cat/tv3/alacarta/tot-es-mou/que-es-loxid-detile-per-que-es-tan-inflamable/video/6008166/

3. "Explosió a la petroquímica: hi va haver núvol tòxic o no?. Interview by Toni Clapés, program "Versió RAC1", RAC1 Radio. January 15th, 2020: https://www.rac1.cat/programes/versio/20200115/472913159085/petroquimica-iqoxe-tarragona-nuvol-toxic-oxid-etile.html

4. "Les petroquímiques són imprescindibles per entendre la vida d'avui". Interview by Robert Calvo, for "La Brúixola" program, Onda Cero Radio. January 15th, 2020: https://www.ondacero.es/emisoras/catalunya/audios-podcast/bruixola/les-petroquimiques-son-imprescindibles-per-entendre-la-vida-davui_202001155e1f9a8c0cf2d11c7c2d33e1.html

5. "Los riesgos para la salud del 5G, la polémica en el Mobile World Congress". Interview by Ignasi Jorro, Cronica Global section of El Español Journal. January 16th, 2020: https://cronicaglobal.elespanol.com/business/ada-colau-mobile-world-congress_309704_102.html

6. "Tres falsos mitos sobre los coches de hidrógeno". Interview by Marta Andreu, Motor Section of La Vanguardia Journal. March 3rd, 2020: https://www.lavanguardia.com/motor/actualidad/20200227/473658774341/3-falsos-mitos-sobre-los-coches-de-hidrogeno-movilidad-futuro-hyundai-electricos.html

7. "El MMS, el dióxido de cloro o el clorito de sodio curan el nuevo coronavirus?". Interview by Miguel Ángel Bravo for AFP Factual, April 17th, 2020: https://factual.afp.com/el-mms-el-dioxido-de-cloro-o-el-clorito-de-sodio-pueden-ser-daninos-para-la-salud-y-no-hay-pruebas

8. "Alertan que el MMS es muy peligroso y no cura la COVID-19". Interview by Mariela León for Cambio16 journal, April 21st, 2020: https://www.cambio16.com/alertan-el-peligro-del-mms-para-combatir-coronavirus/

9. 81. "El teletreball: un abans i un després per a la contaminació a Barcelona". Interview by Adrià Lizanda for Tot Barcelona digital journal, April 25th, 2020: https://www.totbarcelona.cat/economia/teletreball-llico-confinament-esperanca-medi-ambient_2121375102.html

9. "La verdad del MMS y CDS. ¿Curan enfermedades? ¿Estafa o panacea? | MMS Parte II | Medicina Clara". Interview by Dr. Fernando Fernández Bueno for Medicina Clara Youtube Channel, May 27th, 2020: https://www.youtube.com/watch?v=5GDv1K9JxK4

10. "¿Puede explotar una botella de gel desinfectante por el calor en el coche?". Interview by Marta Andreu for Motor Section, La Vanguardia journal, June 2nd, 2020 https://www.lavanguardia.com/motor/actualidad/20200602/481393338430/puede-explotar-hidrogel-calor-coche-incendio-foto-desescalada-confinamiento-coronavirus-covid-19.html

11. "¿Puede explotar la batería de un patinete eléctrico?". Interview by Marta Andreu for Motor Section, La Vanguardia journal, July 22nd, 2020: https://www.lavanguardia.com/motor/actualidad/20200722/482326177940/puede-explotar-bateria-patinete-electrico-incendio.html

12. "No, el dióxid de clor i el MMS no curen el Coronavirus". Interview by Martí Odriozola for Verificat.cat digital journal, August 4th, 2020: https://www.verificat.cat/fact-check/no-el-dioxid-de-clor-i-lmms-no-curen-el-coronavirus

13. "L'MMS, medicament miraculós". Interview by Alba Tobella for Fact–checking Section, Aquí amb Josep Cuní program, SER Catalunya Radio, August 7th, 2020: https://play.cadenaser.com/audio/1596789138261/

14. "Un laser para medir la atmósfera". Interview by Leyre Flemerique, Big Vang section of La Vanguardia Journal, August 21st, 2020: https://www.lavanguardia.com/ciencia/20200811/482787188405/laser-rayo-atmosfera-concordia-antartida-lidar.html

15. "Verdades y mentiras sobre el dióxido de cloro". Interview By Claudia Chávez for Ojo-Público digital journal, Perú, September 23rd, 2020: https://ojo-publico.com/2116/mitos-y-verdades-sobre-el-uso-del-dioxido-de-cloro

16. "Cómo evitar contagios de la Covid–19 por aerosoles en el coche". Interview by Marta Andreu for La Vanguardia journal, Moveo Section, October 21st, 2020: https://www.lavanguardia.com/motor/consejos/20201021/33867/como-evitar-contagios-covid-19-aerosoles-coche.html

17. "El dióxido de cloro no debe ingerirse pero puede usarse como desinfectante contra la Covid–19". Interview by Natalia Sanguino for AFP Factual España digital press agency, Madrid, November 4th, 2020: https://factual.afp.com/el-dioxido-de-cloro-no-debe-ingerirse-pero-puede-usarse-como-desinfectante-contra-el-covid-19

18. “Els fogons, forns i estufes de gas suposen risc encara que no hi hagi mala combustió”. Interview by Victor Endrino for RAC1 digital edition, December 10, 2020: https://www.rac1.cat/societat/20201210/491028602935/gas-natural-butano-llar-de-foc-combustio-riscos-perills-forn-fogons-estufa.html

II.2 IQTCUB SEMINARS AND CONFERENCES

During 2020 Dr. Carles Curutchet and Dr. Jordi Poater have organized the following IQCT's seminars and conferences:

1. **Dr. Paul Bagus** (University of North Texas) Denton, USA.
   Golden years in the development of Quantum Chemistry at Chicago (LMSS) and San Jose (IBM): Lessons that are relevant today.
   22 January 2020.

2. **Dr. Eduard Matito** (Donostia International Physics Center, DIPC), Donosti, Spain.
   Singling out dynamic and nondynamic correlation
   25 February 2020.

3. **Dr. Pablo Ordejón** (ICN2), Barcelona, Spain.
   Computing the properties of materials and devices from first principles: 25 years of SIESTA
   9 October 2020.

II.3 IQTCUB INVITED RESEARCHERS

During 2020, a total of seven researchers have spent some time at the IQTCUB collaborating in different research projects.

1. **MSc. Masoomeh Keyhanian** (invited researcher).
   University of Mazandaran, Iran.
   January-December 2020.

2. **MSc. Hedda Oschinski** (ERASMUS program researcher)
   Leibniz University, Germany.
   January-march 2020.

3. **Nicola Danielis** (invited researcher).
   University of Trieste, Italy.
   January-april 2020.

4. **Enrico Bisquoli** (invited researcher).
   University of Pisa, Italy.
   January-june 2020.

5. **MSc. Lizzie Sargeant** (HPC Europe researcher).
   Birmingham University, United Kingdom.
   July-September 2020.

6. **Alberto Pérez de Alba Ortiz** (invited researcher).
   University of Amsterdam, Netherlands.
   August-October 2020.

7. **Ferran Nieto Fabregat** (invited researcher)
   University of Naples, Italy.
   September-December 2020.

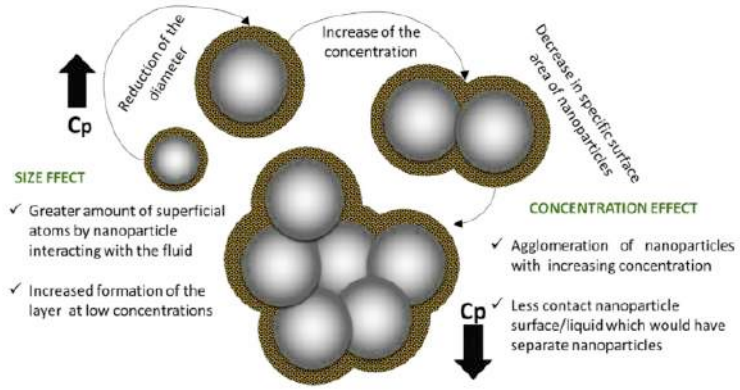
III. SCIENTIFIC ACTIVITY OF IQTCUB MEMBERS

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

Effect of nanoparticles in molten salts – MD simulations and experimental study.
A.Svobodova-Sedlackova, C. Barreneche, G. Alonso, A. I. Fernández, P. Gamallo.
Renew. Energy, *152* (2020) 208-216.



Main parameters that affect thermal capacity: concentration and size of nanoparticles in the nanofluid.

Experimental studies on nanofluids reveal an anomalous increment in the specific heat capacity of these ionic systems when nanoparticles are added. This fact is really important due the applicability of nanofluids in concentrating solar power plants as heat transfer fluid and storage media. These are promising results for the development of high-temperature heat storage applications by enhanced storage capacity materials. We have studied the effect of SiO_2 nanoparticles in $NaNO_3$ molten salt by molecular dynamics (MD) simulations and Differential Scanning Calorimetry (DSC) experiments. The study shows that for nanoparticles' concentrations around 1% wt. the C_p increases by 26% compared to pure $NaNO_3$, whereas at higher concentrations the effect disappears.

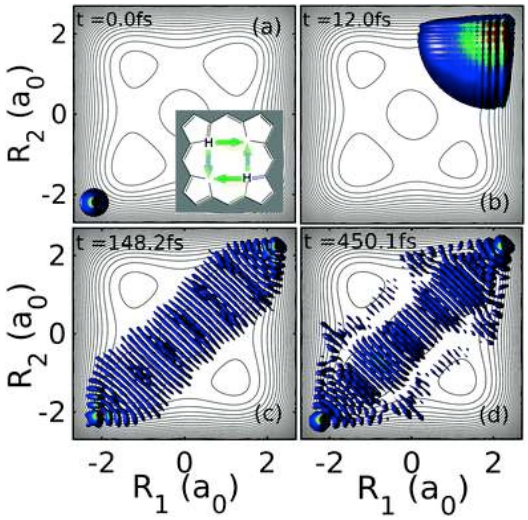
Multiscale study of the mechanism of catalytic CO_2 hydrogenation: role of the Ni(111) facets.

P. Lozano-Reis, H. Prats, P. Gamallo, F. Illas, R. Sayós.

ACS Catal., *10* (2020) 8077-8089.

The molecular mechanism of CO_2 hydrogenation on a Ni(111) surface has been investigated by means of periodic density functional theory calculations, including dispersion interactions, along with accurate kinetic Monte Carlo simulations, including lateral interactions between the adsorbates. The present reaction model involves 25 different species and a total of 86 elementary processes, including adsorptions, desorptions, surface chemical steps, and diffusions. The reaction network accounts for three different mechanisms for the reverse water-gas shift reaction and three different mechanisms for methanation. The kinetic Monte Carlo simulations reveal that the reverse water-gas shift reaction dominates the CO_2 hydrogenation on Ni(111) with no evidence of methane formation. The reaction proceeds mainly through the redox route, with the carboxyl pathway also being active but to a lesser extent.

Quantum equilibration of the double-proton transfer in a model system porphine.
G. Albareda, A. Riera, M. González, J. M. Bofill, I. P. R. Moreira, R. Valero, I. Tavernelli.
Phys. Chem. Chem. Phys., *22* (2020) 22332.



Two-proton probability density at four representative time values. The initially well-localized nuclear density gives way later to a strong proton delocalization along the synchronous pathway that is maintained for at least 1 ps.

There is a renewed interest in the derivation of statistical mechanics from the dynamics of closed quantum systems. A central part of this program is to understand how closed quantum systems initialized far-from-equilibrium can share a dynamics that is typical to the relaxation towards thermal equilibrium. We consider here the equilibration of a two-dimensional model describing the double proton transfer reaction in porphine. From quantum dynamics simulations it comes out that equilibration takes place very rapidly (∼200 fs) for initial states with energies well above the synchronous barrier. The resulting equilibration state shows a strong delocalization of the protons probability density which arises from: (i) an initial state consisting of a large superposition of vibrational states; (ii) the presence of a very effective dephasing mechanism. This work, which involves two groups of IQTC and was led by Dr. Guillem Albareda, was selected as “2020 PCCP Hot Article”.

MXenes as promising catalysts for water dissociation.

J. D. Gouveia, Á. Morales-García, F. Viñes, F. Illas, J. R. B Gomes.

Appl. Catal. B 260 (2020) 118191.

MXenes effectively dissociate water suggesting them as catalysts for industrially relevant processes such as the water-gas shift reaction.

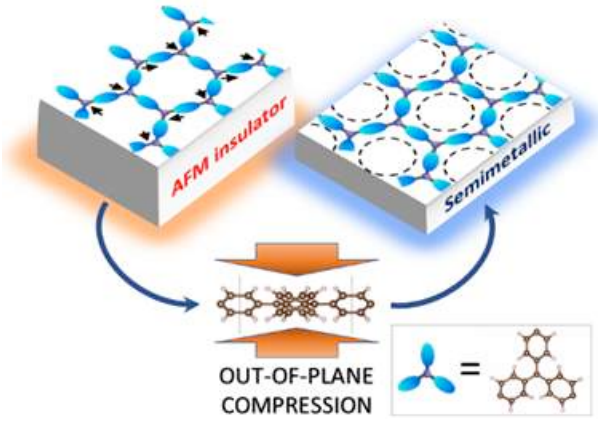
Investigation based on density functional theory report that M_2X (M=Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, and W, while X=C or N) MXenes exothermically adsorb water and greatly facilitate its dissociation, with low energy barriers. This work shows the possible application of MXenes as heterogeneous catalysts for water dissociation, effectively suggesting their potential in relevant processes such as the water-gas shift reaction.

LINE 2. NANOMATERIALS AND NANOELECTRONICS

2D Hexagonal covalent organic radical frameworks as tunable correlated electron systems.

R. Santiago Piera, I. Alcon, J. Ribas Ariño, M. Deumal, I. P. R. Moreira, S. T. Bromley.

Adv. Funct. Mater., *31* (2020) 2004584.

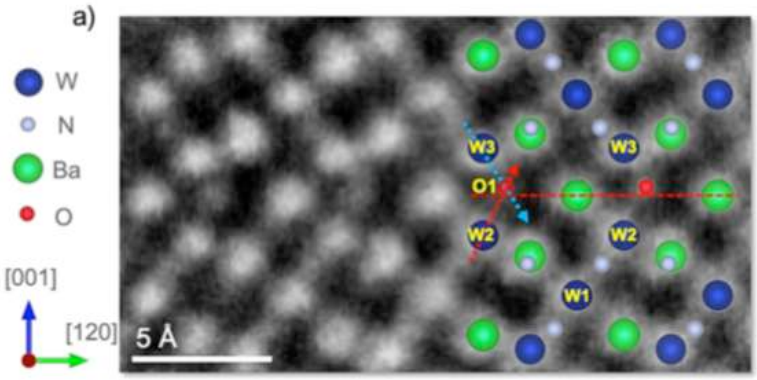


The study shows that electron correlation can be simply tuned in experimentally viable 2D hexagonally ordered covalent organic radical frameworks (2D hex-CORFs) and thus establishes them as a class of versatile single-layer quantum materials.

Engineering polar oxynitrides: hexagonal perovskite $BaWON_2$.

J. Oró-Solé, I. Fina, C. Frontera, J. Gàzquez, C. Ritter, M. Cunquero, P. Loza-Alvarez, S. Conejeros, P. Alemany, E. Canadell, J. Fontcuberta, A. Fuertes.

Angew. Chem. Int. Ed., *59* (2020) 1-6.



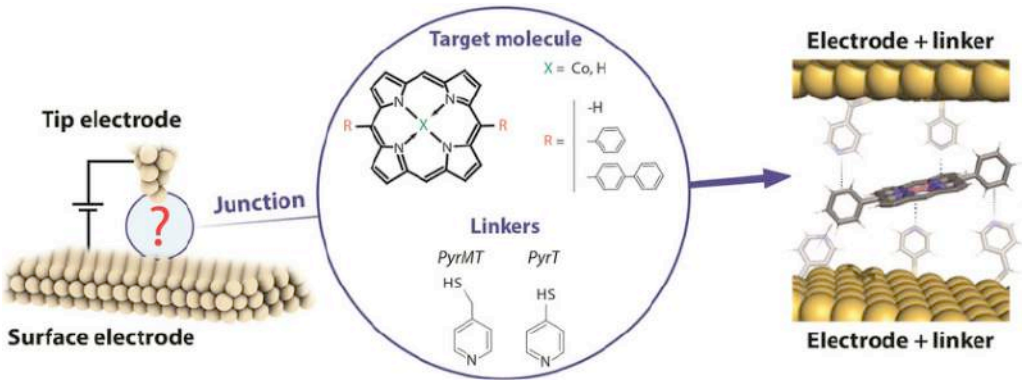
Atomic resolution scanning transmission electron microscopy image of $BaWON_2$ viewed along a-axis. The superimposed structure corresponds to the P63mc model refined from Synchrotron X-ray diffraction.

Known perovskite oxynitrides show centrosymmetric structures, and for some of them high permittivities have been observed and ascribed to local dipoles induced by partial order of nitride and oxide. We report here on the first hexagonal perovskite oxynitride $BaWON_2$, which shows a polar 6H polytype. Synchrotron X-ray and neutron powder diffraction, and annular bright-field in scanning transmission electron microscopy indicate that it crystalizes in the non-centrosymmetric space group $P6_3mc$, with a total order of nitride and oxide at two distinct coordination environments in cubic and hexagonal packed BaX_3 layers. A synergetic second-order Jahn–Teller effect, supported by first principle calculations, anion order, and electrostatic repulsions between W^{6+} cations, induce large distortions at two inequivalent face-sharing octahedra that lead to long-range ordered dipoles and spontaneous polarization along the c axis.

Tuning Single-Molecule Conductance in Metalloporphyrin-Based Wires via Supramolecular Interactions.

A. C. Aragonès, A. Martin-Rodríguez, D. Aravena, J. Puigmartí-Luis, D. B. Amabilino, N. Aliaga-Alcalde, A. Gonzalez-Campo, E. Ruiz, I. Díez-Pérez.

Angew. Chem. Int. Ed., *59* (2020) 19193-19201.

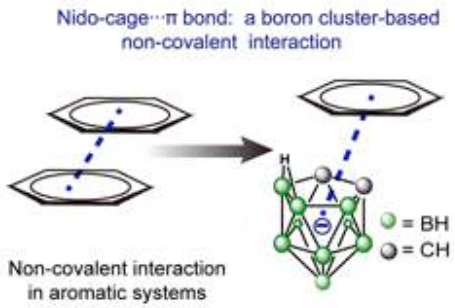


Nature has developed supramolecular constructs to deliver outstanding charge-transport capabilities using metalloporphyrin-based supramolecular arrays. Herein we incorporate simple, naturally inspired supramolecular interactions via the axial complexation of metalloporphyrins into the formation of a single-molecule wire in a nanoscale gap. Small structural changes in the axial coordinating linkers result in dramatic changes in the transport properties of the metalloporphyrin-based wire. The increased flexibility of a pyridine-4-yl-methanethiol ligand due to an extra methyl group, as compared to a more rigid 4-pyridinethiol linker, allows the pyridine-4-yl-methanethiol ligand to adopt an unexpected highly conductive stacked structure between the two junction electrodes and the metalloporphyrin ring. DFT calculations reveal a molecular junction structure composed of a shifted stack of the two pyridinic linkers and the metalloporphyrin ring. In contrast, the more rigid 4-mercaptopyridine ligand presents a more classical lifted octahedral coordination of the metalloporphyrin metal center, leading to a longer electron pathway of lower conductance.

Nido-Cage···pi bond: a non-covalent interaction between boron clusters and aromatic rings and its applications.

H. Yan, D. Tu, J. Poater, M. Solà.

Angew. Chem. Int. Ed., *59* (2020) 9018-9025.

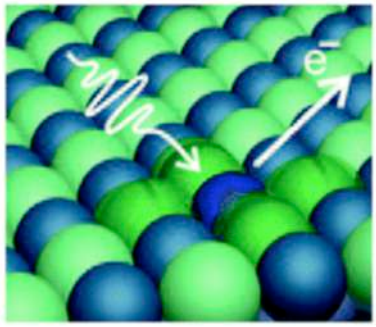


Non-covalent interactions involving multicenter multielectron skeletons such as boron clusters are rare. Now, a non-covalent interaction, the nido-cage···π bond, is discovered based on the boron cluster $C_2B_9H_{12}^-$ and an aromatic π system. The X-ray diffraction studies indicate that the nido-cage···π bonding presents parallel-displaced or T-shaped geometries. The contacting distance between cage and π ring varies with the type and the substituent of the aromatic ring. Theoretical calculations reveal that this nido-cage···π bond shares a similar nature to the conventional anion···π or π···π bonds found in classical aromatic ring systems. This nido-cage···π interaction induces variable photophysical properties such as aggregation-induced emission and aggregation-caused quenching in one molecule. This work offers an overall understanding towards the boron cluster-based non-covalent bond and opens a door to investigate its properties.

Limitations of the equivalent core model for understanding core-level spectroscopies.

P. S. Bagus, C. Sousa, F. Illas.

Phys. Chem. Chem. Phys. 22 (2020) 22617.



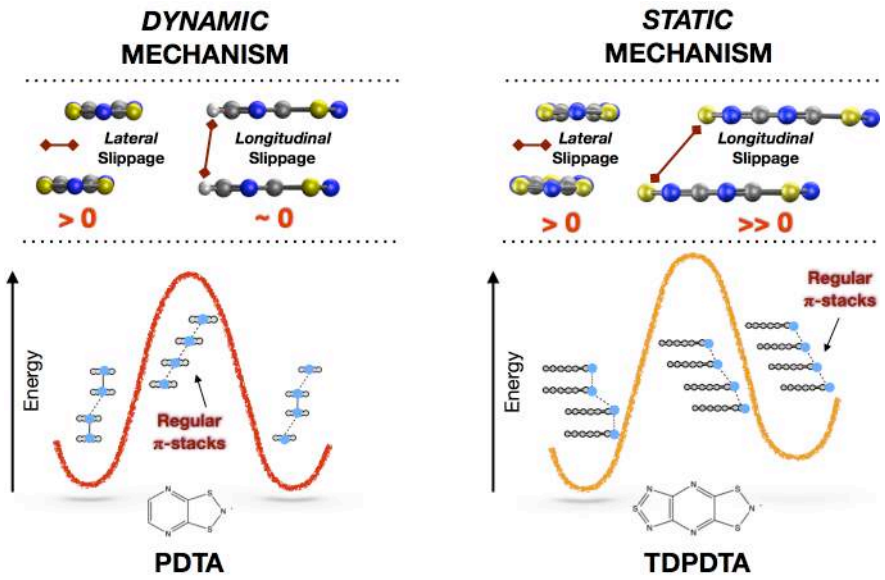
Scheme of the light absorbance and electron excitaiton on a surface, addressed here by the core-hole theory and the equivalent core model.

In the present study a detailed comparison of the electronic structure provided from rigorous core-hole theory and from the equivalent core, Z + 1 approximation, is carried out to assess the latter validity and the utility, revealing a qualitative view of initial and core-hole electronic structures, yet fails distinguishing between initial and final state contributions to the binding energy shifts, with the concomitant threat of incorrectly assigning them, as the Z + 1 model stresses the role of final state effects.

Two different mechanisms of stabilization of regular p-stacks of radicals in switchable dithiazolyl-based materials.

T. Francese, S. Vela, M. Deumal, F. Mota, J.J. Novoa, M. Farnesi Camellone, S. Fabris, R.W.A. Havenith, R. Broer, J. Ribas-Arino.

J. Mater. Chem. C., *8* (2020) 5437.

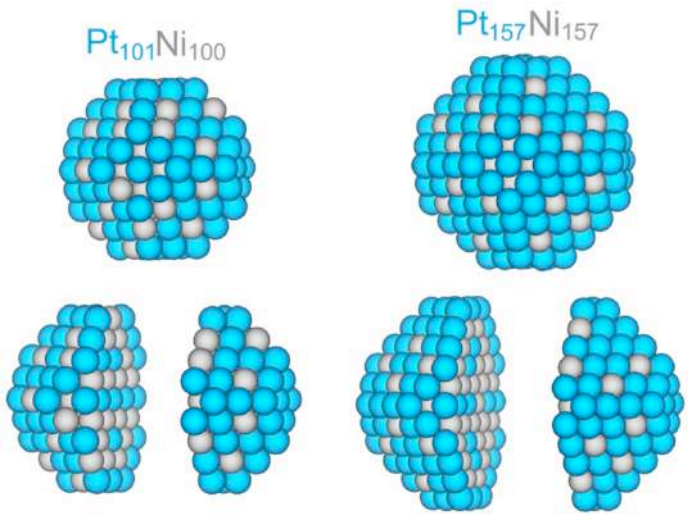


Materials based on regular π-stacks of planar organic radicals are intensively pursued by virtue of their technologically relevant properties. Yet, these π-stacks are commonly unstable against π-dimerization. In this computational study, we reveal that regular π-stacks of planar dithiazolyl radicals can be rendered stable, in some range of temperatures, via two different mechanisms. When the radicals of a π-stack are both longitudinally and latitudinally slipped with respect to each other, the corresponding regular π-stacked configuration is associated with a locally stable minimum in the potential energy surface of the system. Conversely, those regular π-stacks in which radicals are latitudinally slipped with respect to each other are stable as a result of a dynamic interconversion between two degenerate dimerized configurations. The existence of two stabilization mechanisms, which can be traced back to the bonding properties of isolated π-dimers, translates into two different ways of exploiting spin-Peierls-like transitions in switchable dithiazolyl-based materials.

Irreversible structural dynamics on the surface of bimetallic PtNi alloy catalyst under alternating oxidizing and reducing environments.

I. Khalakhan, L. Vega, M. Vorokhta, T. Skála, F. Viñes, Y. V. Yakovlev, K. M. Neyman, I. Matolínová.

Appl. Catal. B: Environ., *264* (2020) 118476.



Calculated equilibrium chemical ordering in 1:1 Pt:Ni nanocrystals containing 201 and 314 atoms.

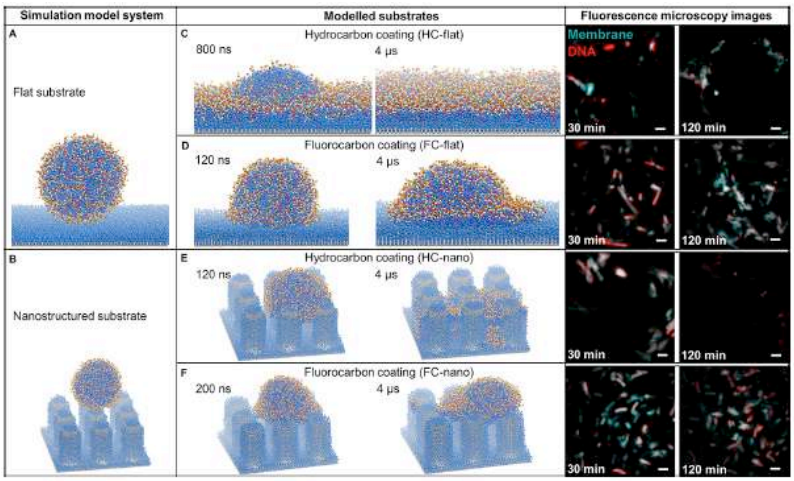
This combined experimental and computational modelling study provides new insights into the PtNi alloy surface chemistry under reactive environments. It allowed gaining advanced understanding of the action of PtNi catalysts at real conditions, including their long-time catalytic performance in fuel cells. The surface segregation of Ni species caused by reactive environments suppresses PtNi alloy on the surface which is critical for its high electrocatalytic performance. Based on the obtained results a general strategy towards adjustment of PtNi catalyst surfaces has been proposed. The redox pre-treatment of the surface of bimetallic catalysts may open an effective way to engineer highly efficient catalysts for various catalytic processes.

LINE 3. BIOMEDICINE AND SOFT MATTER

Direct and fast assessment of antimicrobial surface activity using molecular dynamics simulation and time-lapse imaging.

R. Sibilo, I. Mannelli, R. Reigada, C. Manzo, M. A. Noyan, P. Mazumder, V. Pruneri.

Anal. Chem., *92* (2020) 6795-6800.

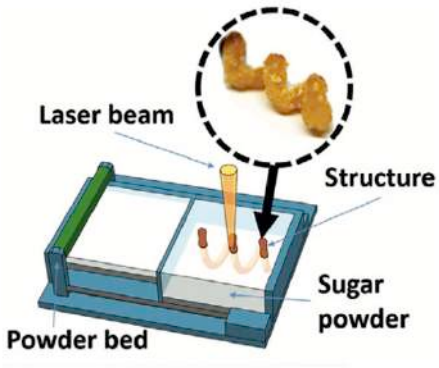


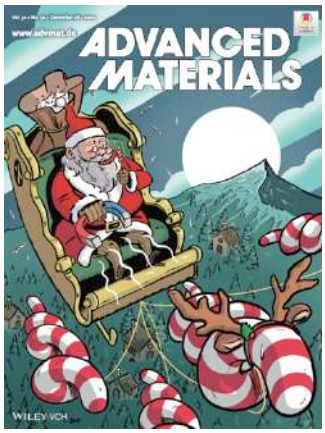
With the alarming rise of antimicrobial resistance, studies on bacteria−surface interactions are both relevant and timely. Scanning electron microscopy and colony forming unit counting are commonly used techniques but require sophisticated sample preparation and long incubation time. Here, we present a direct method based on molecular dynamics simulations of nanostructured surfaces providing in silico predictions, complemented with time-lapse fluorescence imaging to study live interactions of bacteria at the membrane− substrate level. We evaluate its effectiveness in predicting and statistically analyzing the temporal evolution and spatial distribution of prototypical bacteria (*E. coli*) on surfaces with nanopillars. We observed cell reorientation, clustering, membrane damage, growth inhibition, and in the extreme case of hydrocarbon-coated nanopillars, this was followed by cell disappearance, validating the obtained simulation results.

CANDYBOTS: a new generation of 3D-printed sugar-based transient small-scale robots.

S. Gervasoni, A. Terzopoulou, C. Franco, A. Veciana, N. Pedrini, J. T. Burri, C. de Marco, E. C. Siringil, X-Zh. Chen, B. J. Nelson, J. Puigmartí-Luis, S. Pané.

Adv. Mater., *32* (2020) 2005652.



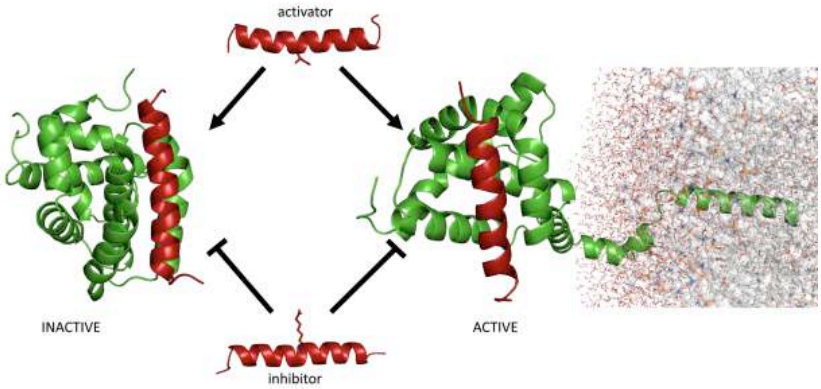


Sugars are among the main sources of energy and structural building blocks for almost all forms of life. Because of their degradability, resorbability, and biocompatibility, sugars are compelling materials in transient devices and robotics. Here, an additive manufacturing approach for the production of sugar-based 3D composites is introduced, which can pave the way for a new generation of transient small-scale devices.

Molecular determinants for the activation/inhibition of bak protein by BH3 peptides.

G. Vila-Julià, J. M. Granadino-Roldán, J. J. Perez , J. Rubio-Martinez.

J. Chem. Inf. Model., *60* (2020) 1631-1643.



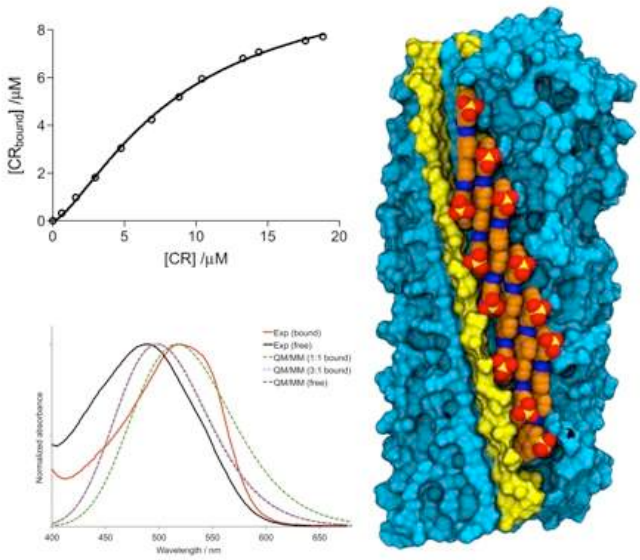
Molecular determinants for the activation/inhibition of Bak protein on its active/inactive conformation by BH3 peptides.

This work reports the results of a computational study aimed to understand the behaviour of the pro-apoptotic protein Bak, which belongs to the Bcl-2 family of proteins. Members of this family share high similarity in structural terms as well as in their binding sites. However, they can act either avoiding or promoting apoptosis. Inactivation of Bak produces an increase of proliferation in many tumours. Thus, determining the binding mechanism of activators to Bak and what regions of the protein are modified during the activation process is key to develop new molecules that are able to mimic these Bak activators, using them as promising strategies in the treatment of tumours that have Bak inactivated.

On the binding of congo red to amyloid fibrils.

A. Espargaró, S. Llabrés, S. J. Saupe, C. Curutchet, F. J. Luque, R. Sabaté**.**

Angew. Chem. Int. Ed. *59* (2020), 8104-8107.



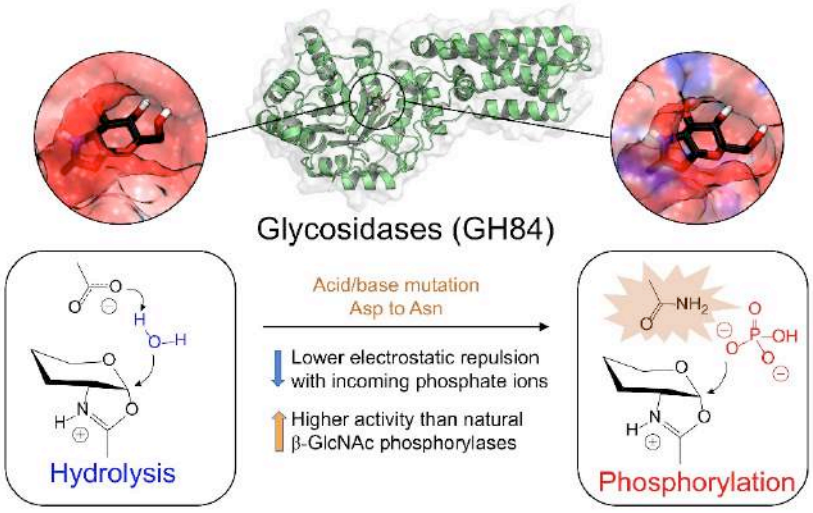
Congo red binds to amyloid fibrils with the long axis oblique to the fibril axis and the plane radial to the fibril core, following a cooperative mechanism characterized by the formation of a 1:1 stoichiometric complex.

Amyloids are characterized by their capacity to bind Congo red (CR), one of the most used amyloid-specific dyes. The structural features of CR binding were unknown for years, mainly because of the lack of amyloid structures solved at high resolution. In the last few years, solid-state NMR spectroscopy enabled the determination of the structural features of amyloids like the HET-s prion forming domain (HET-s PFD) and its binding by CR. In this study, spectroscopic data was combined with molecular docking, molecular dynamics, and excitonic quantum/molecular mechanics calculations to examine and rationalize CR binding to amyloids. In contrast to a previous assumption on the binding mode, the results indicated that CR binding to the HET-s PFD involves a cooperative process entailing the formation of a complex with 1:1 stoichiometry.

A single point mutation converts GH84 *O*-GlcNAc hydrolases into phosphorylases. Experimental and theoretical evidence.

D. Tezé, J. Coines, L. Raich, V. Kalichuk, C. Solleux, C. Tellier, C. André-Miral, B. Svensson, C. Rovira.

J. Am. Chem. Soc., *142* (2020) 2120.

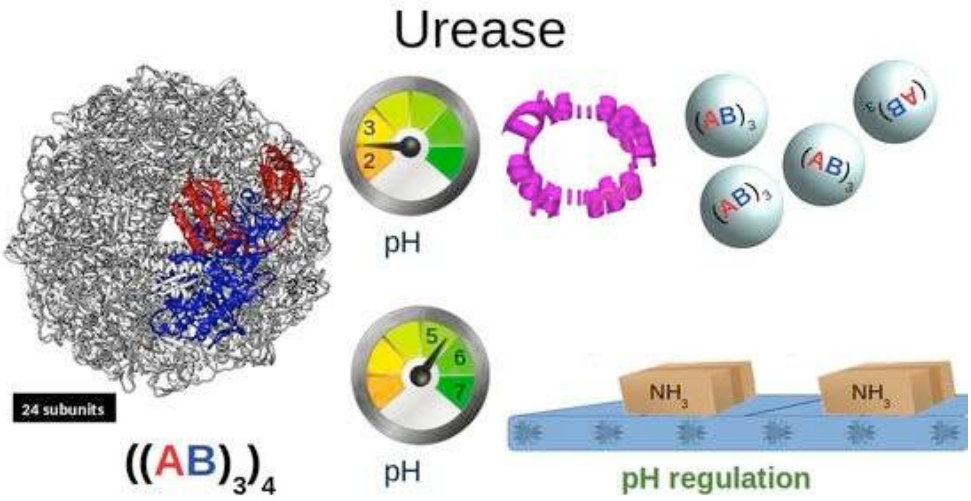


Glycoside hydrolases (GHs) and phosphorylases (GPs) are two major classes of enzymes responsible for the break down of carbohydrates in nature. Here we showed that two GHs (in particular, two *O*-glucosaminyl glucosidases) can be converted to efficient phosphorylases just by the replacement of an amino acid in the enzyme active site (Asp120Asn single point mutation). Using molecular dynamics and QM/MM metadynamics methods we show that the mutation changes the electrostatic potential at the active site and drastically reduces the energy barrier for phosphorolysis, which becomes favoured over hydrolysis. Noteworthy, kinetic experiments show that the mutated enzymes are over 10-fold more active than their corresponding naturally occurring phosphorylases. These insights expand our understanding of GH and GP mechanisms, providing a basis for the generation of enzymatic variants that could be amenable for the large scale production of valuable phosphorylated glycosides.

Effect of pH on the supramolecular structure of helicobacter pylori urease by molecular dynamics simulations.

H. L. Barazorda-Ccahuana, B. Gómez, F. Mas, S. Madurga.

Polymers, *12* (2020) 2713.



Ammonia production from *Helicobacter pylori* urease allows the pH of the environment to be regulated. At very acidic pHs protein denaturation occurs.

The effect of pH on the supramolecular structure of *Helicobacter pylori* urease was studied by means of molecular dynamics simulations at seven different pHs. Appropriate urease charge distributions were calculated using a semi-grand canonical Monte Carlo (SGCMC) procedure that assigns each residue's charge state depending on the assigned individual pKa obtained by PROPKA. The effect of pH on protein stability has been analyzed through root-mean-square deviation (RMSD), radius of gyration, solvent-accessible surface area, hydrogen bonds and salt bridges. Urease catalyses the hydrolysis of urea in 12 active sites that are covered by mobile regions that act like flaps. The mobility of these flaps is increased at acidic pHs. However, extreme acidic conditions cause urease to have the least number of stabilizing interactions. This initiates the process of denaturalization, wherein the four $(\alpha\beta)_3$ subunits of the global structure $((\alpha\beta)_3)_4$ of urease start to separate.

III.2 PUBLICATION LIST

PUBLISHED ARTICLES

1. *First-Principles calculations on the adsorption behavior of amino acids on a titanium carbide MXene.*
J. D. Gouveia, G. Novell-Leruth, P. M. L. S. Reis, F. Viñes, F. Illas, J. R. B. Gomes.
ACS Appl. Bio Mater. *11* (2020) 8437.

2. *Unravelling the surface chemistry and structure in highly active sputtered Pt_3Y catalyst films for the oxygen reduction reaction.*
R. Brown, M. Vorokhta, I. Khalakhan, M. Dopita, T. Vonderach, T. Skála, N. Lindahl, I. Matolinová, H. Grönbeck, K. M. Neyman, V. Matolin, B. Wickman.
ACS Appl. Mater. Inter. *12* (2020) 4454-4463.

3. *Enhancing CO_2 electroreduction to ethanol on copper-silver composites by opening an alternative catalytic pathway.*
L. R. L. Ting, O. Piqué, S. Y. Lim, M. Tanhaei, F. Calle-Vallejo, B. S. Yeo.
ACS Catal. *10* (2020) 4059.

4. *Facile heterogeneously catalyzed nitrogen fixation by MXenes.*
J. D. Gouveia, Á. Morales-García, F. Viñes, J. R. B. Gomes, F. Illas.
ACS Catal. *10* (2020) 5049.

5. *A semiempirical method to detect and correct DFT-based gas-phase errors and its application in electrocatalysis.*
L. P. Grande-Marulanda, A. Rendón-Calle, S. Builes, F. Illas, M. T. M. Koper, F. Calle-Vallejo.
ACS Catal. *10* (2020) 6900.

6. *Critical hydrogen coverage effect on the hydrogenation of ethylene catalyzed by δ-MoC(001): an ab initio thermodynamic and kinetic study.*
C. Jimenez-Orozco, E. Flórez, F. Viñes, J. A. Rodriguez, F. Illas.
ACS Catal. *10* (2020) 6213.

7. *Multiscale study of the mechanism of catalytic CO_2 hydrogenation: role of the Ni(111) facets.*
P. Lozano-Reis, H. Prats, P. Gamallo, F. Illas, R. Sayós.
ACS Catal. *10* (2020) 8077.

8. *Substrate engagement and catalytic mechanisms of N-acetylglucosaminyltransferase.*
V. J. Darby, A. K. Gilio, B. Piniello, C. Roth, E. Blagova, R. Hubbard, C. Rovira, G. J. Davies, L. Wu.
ACS Catal. *10* (2020) 8590−8596.

9. *Elucidating the structure of ethanol-producing active sites at oxide-derived Cu electrocatalysts.*
O. Piqué, F. Viñes, F. Illas, F. Calle-Vallejo.
ACS Catal. *10* (2020) 10488.

10. *The catalytic reaction mechanism of the β-galactocerebrosidase enzyme deficient in Krabbe disease.*
A. Nin-Hill, C. Rovira.
ACS Catal. *10* (2020) 12091-12097.

11. *Activation of O_2 and H_2O_2 by lytic polysaccharide monooxygenases.*
B. Wang, Z. Wang, G. J. Davies, P. H. Walton, C. Rovira.
ACS Catal. *10* (2020) 12760-12769.

12. *MXenes: new horizons in catalysis.*
Á. Morales-García, F. Calle-Vallejo, F. Illas.
ACS Catal. *10* (2020) 13487.

13. *An epoxide intermediate in glycosidase catalysis.*
L. F. Sobala, G. Speciale, S. Zhu, L. Raich, N. Sannikova, A. J. Thompson, Z. Hakki, D. Lu, Y. Zhang, S. S. K. Abadi, A. R. Lewis, V. Rojas-Cervellera, G. Bernardo-Seisdedos, O. Millet, J. Jiménez-Barbero, A. J. Bennet, M. Sollogoub, C. Rovira, G. J Davies, S. J. Williams.
ACS Cent. Sci. *6* (2020) 760-770.

14. *Vibrational analysis of manganese(II) oxalates hydrates: an in silico statistical approach.*
H. L. Barazorda-Ccahuana, M. Nedyalkova, I. Kichev, S. Madurga, B. Donkova, V. Simeonov.
ACS Omega *5* (2020) 9071-9077.

15. *New insights about the structural properties of κ-(BEDT-TTF)$_2$X$_2$(CN)$_3$ (X=Cu and Ag) spin liquids.*
P. Foury-Leylekian, V. Ilakovac, P. Fertey, V. Balédent, O. Milat, K. Miyagawa, K. Kanoda, T. Hiramatsu, Y. Yoshida, G. Saito, P. Alemany, E. Canadell, S. Tomic, J.-P. Pouget.
Acta Cryst. *B76* (2020) 581-590.

16. *Microfluidic-assisted blade coating of compositional libraries for combinatorial applications: the case of organic photovoltaics.*
X. Rodríguez-Martínez, S. Sevim, X. Xu, C. Franco, P. Pamies-Puig, L. Córcoles-Guija, R. Rodriguez-Trujillo, F. Javier del Campo, D. Rodríguez-San-Miguel, A. deMello, S. Pané, D. B. Amabilino, O. Inganäs, J. Puigmartí-Luis, M. Campoy-Quiles.
Adv. Energy Mater. *10* (2020) 2001308.

17. *3D-printed soft magnetoelectric microswimmers for delivery and differentiation of neuron-like cells.*
M. Dong, X. Wang, X.-Z. Chen, F. Mushtaq, S. Deng, C. Zhu, H. Torlakcik, A. Terzopoulou, X.-H. Qin, X. Xiao, J. Puigmartí-Luis, H. Choi, Q.-D. Shen, B. J. Nelson, S. Pané.
Adv. Funct. Mater. *30* (2020) 1910323.

18. *2D hexagonal covalent organic radical frameworks as tunable correlated electron systems.*
R. Santiago, I. Alcón, J. Ribas-Ariño, M. Deumal, I. d. P. R. Moreira, S. T. Bromley.
Adv. Funct. Mater. (2020) 2004584.

19. *Enhancing long-term device stability using thin film blends of small molecule semiconductors and insulating polymers to trap surface-induced polymorphs.*
T. Salzillo, A. Campos, A. Babuji, R. Santiago, S. T. Bromley, C. Ocal, E. Barrena, R. Jouclas, C. Ruzie, G. Schweicher, Y. H. Geerts, M. Mas-Torrent.
Adv. Funct. Mater. *30* (2020) 2006115.

20. *Biodegradable metal–organic framework-based microrobots (MOFBOTs).*
A. Terzopoulou, X. Wang, X-Zh. Chen, M. Palacios-Corella, C. Pujante, J. Herrero-Martín, Dr. X-H. Qin, J. Sort, A. J. deMello, B. J. Nelson, J. Puigmartí-Luis, S. Pané.
Adv. Healthcare Mater. *9* (2020) 2001031.

21. *In search of chiral molecular superconductors: κ-[(S,S)-DM-BEDT-TTF]$_2$ClO$_4$ revisited.*
N. Mroweh, C. Mézière, F. Pop, P. Auban-Senzier, P. Alemany, E. Canadell, N. Avarvari.
Adv. Mater. *32* (2020) 2002811.

22. *CANDYBOTS: a new generation of 3D-printed sugar-based transient small-scale robots.*
S. Gervasoni, A. Terzopoulou, C. Franco, A. Veciana, N. Pedrini, J. T. Burri, C. de Marco, E. C. Siringil, X-Zh. Chen, B. J. Nelson, J. Puigmartí-Luis, S. Pané.
Adv. Mater. *32* (2020) 2005652.

23. *SERS barcode libraries: a microfluidic approach.*
S. Sevim, A. Sorrenti, S. Pané, A. J. deMello, J. Puigmartí-Luis.
Adv. Sci. *7* (2020) 1903172.

24. *Direct and fast assessment of antimicrobial surface activity using molecular dynamics simulation and time-lapse imaging.*
R. Sibilo, I. Mannelli, R. Reigada, C. Manzo, M. A. Noyan, P. Mazumder, V. Pruneri.
Anal. Chem. *92* (2020) 6795-6800.

25. *Engineering polar oxynitrides: hexagonal perovskite BaWON$_2$.*
J. Oró-Solé, I. Fina, C. Frontera, J. Gàzquez, C. Ritter, M. Cunquero, P. Loza-Alvarez, S. Conejeros, P. Alemany, E. Canadell, J. Fontcuberta, A. Fuertes.
Angew. Chem. Int. Ed. *59* (2020) 1-6.

26. *On the binding of congo red to amyloid fibrils.*
A. Espargaró, S. Llabrés, S. J. Saupe, C. Curutchet, F. J. Luque, R. Sabaté.
Angew. Chem. Int. Ed. *59* (2020) 8104-8107.

27. *The nido-cage···pi bond: a non-covalent interaction between boron clusters and aromatic rings and its applications.*
H. Yan, D. Tu, J. Poater, M. Solà.
Angew. Chem. Int. Ed. *59* (2020) 9018-9025.

28. *Tuning single-molecule conductance in metalloporphyrin-based wires via supramolecular interactions.*
A. C. Aragonès, A. Martin-Rodríguez, D. Aravena, J. Puigmartí-Luis, D. B. Amabilino, N. Aliaga-Alcalde, A. Gonzalez-Campo, E. Ruiz, I. Díez-Pérez.
Angew. Chem. Int. Ed. *59* (2020) 19193-19201.

29. *Dioxygen binding and sensing proteins.*
D. A. Estrín, F. J. Luque, G. Ilangovan, J. L. Zweier.
Antioxid. Redox Signal. *32* (2020) 1151-1154.

30. *MXenes as promising catalysts for water dissociation.*
J. D. Gouveia, A. Morales-García, F. Viñes, F. Illas, J. R. B. Gomes.
Appl. Catal. B *260* (2020) 118191.

31. *Irreversible structural dynamics on the surface of bimetallic PtNi alloy catalyst under alternating oxidizing and reducing environments.*
I. Khalakhan, L. Vega, M. Vorokhta, T. Skála, F. Viñes, Y. V. Yakovlev, K. M. Neyman, I. Matolínová.
Appl. Catal. B *264* (2020) 118476.

32. *Critical effect of carbon vacancies on the reverse water gas shift reaction over vanadium carbide catalysts.*
A. Pajares, H. Prats, A. Romero, P. Ramírez de la Piscina, R. Sayós, N. Homs, F. Illas.
Appl. Catal. B *267* (2020) 118719.

33. *Substantial improvement of electrocatalytic predictions by systematic assessment of solvent effects on adsorption energies.*
A. Rendón-Calle, S. Builes, F. Calle-Vallejo.
Appl. Catal. B *276* (2020) 119147.

34. *Exploiting electrolyte confinement effects for the electrosynthesis of two-engine micromachines.*
M. Fernández-Barcia, B. Jang, Carlos C. J. Alcântara, U. Wolff, A. Gebert, M. Uhlemann, X. Chen, J. Puigmartí-Luis, J. Sort, E. Pellicer, S. Pané.
App. Mater. Today *19* (2020) 100629.

35. *Pathway selection as a tool for crystal defect engineering: s case study with a functional coordination polymer.*
A. Abrishamkar, S. Suárez–García, S. Sevim, Sh-X. Liu, S. Decurtins, G. Aromí, D. Aguilà, S.Pané, A. J. deMello, A. Rotaru, D. Ruiz–Molina, J. Puigmartí-Luis.
App. Mater. Today *20* (2020) 100632.

36. *The nano gold rush: graphynes as atomic sieves for coinage and Pt-group transition metals.*
S. Kim, P. Gamallo, F. Viñes, J. Y. Lee.
Appl. Surf. Sci. *499* (2020) 143927.

37. *Towards understanding the role of carbon atoms of transition metal surfaces: implications for catalysis.*
B. Martínez, O. Piqué, H. Prats, F. Viñes, F. Illas.
Appl. Surf. Sci. *513* (2020) 145765.

38. *Structural and kinetic features of aldehyde dehydrogenase 1A (ALDH1A) subfamily members, cancer stem markers active in retinoic acid biosynthesis.*
R. Pequerul, J. Vera, J. Giménez-Dejoz, I. Crespo, J. Coines, S. Porté, C. Rovira, X. Parés, J. Farrés.
Arch. Biochem. Biophys. *681* (2020) 108256.

39. *Assessing the viability of silicate nanoclusters as carriers of the anomalous microwave emission: a quantum mechanical study.*
A. M. Escatllar, S. T. Bromley.
Astron. Astrophys. *634* (2020) A77.

40. *Insights into the effect of the membrane environment on the three-dimensional structure-function relationship of antimicrobial peptides.*
W. J. Zamora, S. De Souza, F. Separovic, F. J. Luque.
Biophys. J. *118* (2020) 263A.

41. *Pharmacology and preclinical validation of a novel anticancer compound targeting PEPCK.*
M. Aragó, J. Moreno-Felici, S. Abás, S. Rodríguez-Arévalo, P. Hyroššová, 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* (2020) 109601.

42. *Orbitals permit the interpretation of core-level spectroscopies in terms of chemistry.*
P. S. Bagus, F. Illas.
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130. *Quantum equilibration of the double-proton transfer in a model system porphine.*
G. Albareda, A. Riera, M. González, J.M. Bofill, I. de P. R. Moreira, R. Valero, I. Tavernelli.
Phys. Chem. Chem. Phys. *22* (2020) 22332-22341.

131. *Limitations of the equivalent core model for understanding core-level spectroscopies.*
P. S. Bagus, C. Sousa, F. Illas.
Phys. Chem. Chem. Phys. *22* (2020) 22617.

132. *Structural, electronic, and magnetic properties of Ni nanoparticles supported on the TiC(001) surface.*
P. Lozano-Reis, R. Sayós, J. A. Rodriguez, F. Illas.
Phys. Chem. Chem. Phys. *22* (2020) 26145.

133. *Preferential location of zirconium dopants in cerium dioxide nanoparticles and effects of doping on their reducibility: a DFT study.*
I. Z. Koleva, H. A. Aleksandrov, K. M. Neyman, G. N. Vayssilov.
Phys. Chem. Chem. Phys. *22* (2020) 26568-26582.

134. *Weak localization competes with the quantum oscillations in a natural electronic superlattice: the case of* $Na_{1.5}(PO_2)_4(WO_3)_{20}$.
K. K. Kolincio, O. Pérez, E. Canadell, P Alemany, E. Duverger-Nédellec, A. Minelli, A. Bosak, A. Pautrat.
Phys. Rev. B. *101* (2020) 161117(R).

135. *MXenes atomic layer stacking phase transitions and their chemical activity.*
J. D. Gouveia, F. Viñes, F. Illas, J. R. B. Gomes.
Phys. Rev. Mater. *4* (2020) 54003.

136. *Comprehensive analysis of the influence of dispersion on group-14 rutile-type solids.*
Á. Morales-García, F. Illas.
Phys. Rev. Mater. *4* (2020) 73601.

137. *Quantum Zermelo problem for general energy resource bounds.*
J. M. Bofill, A. Sanz, G. Albareda, I. de P.R. Moreira, W. Quapp.
Phys. Rev. Res. *2* (2020) 033492-033502.

138. *Assessing* $Cu_2L_2X_4$ *dimeric moieties as ferromagnetic building blocks in double halide-bridged polymers (X = Cl−, Br− and L = benzamide). An experimental and computational study.*
S. Coetze, M. M. Turnbull, C. P. Landee, J. J. Novoa, M. Deumal, S. Vela, M. Rademeyer.
Polyhedron *185* (2020) 114603.

139. *Crystallization induced enhanced emission in two new Zn(II) and Cd(II) supramolecular coordination complexes with the 1-(3,4-Dimethylphenyl)-5-Methyl-1H-1,2,3-Triazole-4-carboxylate ligand.*
P. Narea, J. Cisterna, A. Cárdenas, P. Amo-Ochoa, F. Zamora, C. Climent, P. Alemany, S. Conejeros, J. Llanos, I. Brito**.**
Polymers *12* (2020) 1756.

140. *Effect of pH on the supramolecular structure of helicobacter pylori urease by molecular dynamics simulations.*
H. L. Barazorda-Ccahuana, B. Gómez, F. Mas, S. Madurga.
Polymers *12* (2020) 2713.

141. *Effect of nanoparticles in molten salts – MD simulations and experimental study.*
A. Svobodova-Sedlackova, C. Barreneche, G. Alonso, A. I. Fernández, P. Gamallo**.**
Renew. Energy *152* (2020) 208.

142. *Single molecule magnets of cobalt and zinc homo- and heterometallic coordination polymers prepared by a one-step synthetic procedure.*
N. Portolés-Gil, S. Gómez-Coca, O. Vallcorba, G. Marbán, N. Aliaga-Alcalde, A. López-Periago, J. A. Ayllón, C. Domingo.
RSC Adv. *10* (2020) 45090-45104.

143. *Structural, electronic and ferroelectric properties of $Zn_{93.75}M_{6.25}O$ (M = Sr, Ba): first-principles calculations.*
H. Hmok, E. Martínez-Aguilar, J. Ribas-Ariño, J. M. Siqueiros Beltrones.
Scr. Mater. *187* (2020) 8-12.

BOOK CHAPTERS AND PROCEEDINGS

1. *Surface structural dynamics in bimetallic PtNi alloy catalyst under simulated operational conditions.*
   I. Khalakhan, L. Vega, M. Vorokhta, T. Skála, F. Viñes, Y. V. Yakovlev, K. M. Neyman, I. Matolínová.
   Elettra Highlights 2019-2020, p.118-119 (Trieste, Italy) 2020.
   www.elettra.eu/science/highlights.html

2. *Magnetically and chemically propelled nanowire-based swimmers.*
   J. Puigmartí-Luis, E. Pellicer, B. Jang, G. Chatzipirpiridis, S. Sevim, X.-Z. Chen, B. J. Nelson, S. Pané.
   Magnetic Nano- and Microwires (Second Edition) edited by M. Vázquez (Woodhead Publishing Series in Electronic and Optical Materials) 2020.

3. *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, USA) 2020.

4. *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) 2020.

5. *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) 2020.

6. *Bohmian Approaches to Non-Adiabatic Molecular Dynamics.*
   G. Albareda, I. Tavernelli.
   Quantum Chemistry and Dynamics of Excited States: Methods and Applications edited by Leticia González, Roland Lindh (John Wiley & Sons, Ltd., USA) 2020.

III.3 OTHER ACTIVITIES

PHD THESES 2020

1. *Catalytic reaction of β-galactocerebrosidase investigated by QM/MM ab initio metadynamics.*
   Alba Nin Hill
   PhD program: Theoretical Chemistry and Computational Modelling.
   Faculty of Chemistry, University of Barcelona.
   Supervisor/s: C. Rovira.
   October 2020.

2. *Computational modelling of TiO_2 and Mg-silicate nanoclusters and nanoparticles - crystallinity and astrophysical implications.*
   Antoni Macià Escatllar
   PhD program: Theoretical Chemistry and Computational Modelling.
   Faculty of Chemistry, University of Barcelona.
   Supervisor/s: Francesc Illas, Stefan T. Bromley.
   September 2020.

3. *Coupling of binding and conformational equilibria in weak polyelectrolytes. Dynamics and charge regulation of biopolymers in crowded media.*
   Pablo M. Blanco Andrés
   PhD program: Theoretical Chemistry and Computational Modelling.
   Faculty of Chemistry, University of Barcelona.
   Supervisor/s: S. Madurga, J. L. Garcés.
   November 2020.

4. *Quantum transport in solid state devices for terahertz frequency applications.*
   Devashish Pandey
   PhD program: Electronics Engineering.
   Electronics Engineering Department, Universitat Autònoma de Barcelona.
   Supervisor/s: G. Alvareda, X. Oriols.
   Desember 2020.

MASTER THESES 2020

1. *Effects of the substituents on the crystal formation and stability of bis-1,2,3-Dithiazolyl radicals. A computational study.*
   Denis Dyatlov
   MSc program: Theoretical Chemistry and Computational Modelling.
   Faculty of Chemistry, University of Barcelona.
   Supervisor/s: Mercè Deumal, Jordi Ribas.
   July 2020.

2. *Mechanical and electronic properties of [1],[2]{1} – grazyne based on DFT calculations.*
   Inga Zhukova
   MSc program: Theoretical Chemistry and Computational Modelling.
   Faculty of Chemistry, University of Barcelona.
   Supervisor/s: Pablo Gamallo.
   July 2020.

3. *Silver and gold nanoalloys: interplay between chemical ordering and optical properties.*
   Nicola Danielis
   MSc program: Corso di Laurea Magistrale in Chimica.
   Dipartimento di Scienze Chimiche e Farmaceutiche, Università di Trieste.
   Supervisor/s: Mauro Stener (Uni. Trieste), Konstantin Neyman.
   July 2020.

4. *Computational investigation of the binding properties of antibacterial photodrugs.*
   Enrico Bisquoli
   MSc program: Corso di Laurea Magistrale in Biotecnologie Molecolari.
   Dipartimento di Biologia, Università di Pisa.
   Supervisor/s: Benedetta Mennucci (Uni. Pisa), Carles Curutchet.
   July 2020.

5. *Computer Aided Assessment of Renewable Resources.*
   Luis Axcel Gutarra Marquina
   MSc program: Environmental Engineering.
   Faculty of Chemistry, University of Barcelona.
   Supervisor/s: J. Bonet, A. E. Plesu.
   July 2020.

6. *Introducing Eco-gamma: a novel environmental impact index for water quantity and quality evaluation.*
   Mauricio Quezada Prado
   MSc program: Environmental Engineering.
   Faculty of Chemistry, University of Barcelona.
   Supervisor/s: J. Bonet, A. E. Plesu.
   July 2020.

7. *Development status of global marine wind energy and contribution to the future development in Spain.*
Marc Llin Brosa
MSc program: Environmental Engineering.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: J. Bonet, A. E. Plesu.
July 2020.

8. *Host-guest interaction in spin-crossover [Fe_4] metal-organic cages.*
Laia Navarro Maestro
MSc program: Atomistic and Multiscale Computational Modelling in Physics, Chemistry and Biochemistry.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: J. Cirera.
July 2020.

9. *Study of structural and electronic properties of spherical TiO_2 nanoparticles by molecular dynamics and DFT calculations.*
Daniel Torrens Gonzalez
MSc program: Theoretical Chemistry and Computational Modelling.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: S. T. Bromley, A. Morales.
July 2020.

10. *Surrogate model for chemical absorbents mixtures for CO_2 capture.*
Antonio Peiró Jiménez
MSc program: Environmental Engineering.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: J. Bonet, A. E. Plesu.
September 2020.

11. *Stretching of hyaluronic acid at the single molecule level.*
Sílvia Sodric Hidalgo
MSc program: Chemistry of Advanced Materials.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: S. Maurga.
September 2020.

12. *Designing new tunable materials for organic electronic devices.*
Kílian Jutglar Lozano
MSc program: Atomistic and Multiscale Computational Modelling in Physics, Chemistry and Biochemistry.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: Stefan Bromley, Jordi Ribas.
September 2020.

13. *Time-optimal control of quantum systems: a solution to the quantum Zermelo problem.*
Lluc Garcia-Gonzalo
MSc program: Photonics.
Faculty of Physics, University of Barcelona.
Supervisor/s: G. Albareda.
October 2020.

SCIENTIFIC CONFERENCES AND MEETINGS 2020

Congreso Internacional y III Congreso Latinoamericano de Química, Física y Biología Computacional
Arequipa (Peru) 20-24 January 2020

Complexation and dynamics of polyelectrolytes in environmental and physiological media
F. Mas, P. M. Blanco, J. L. Garcés, S. Madurga

Simulation and prediction of properties of polyelectrolytes and proteins
S. Madurga, H. L. Barazorda-Ccahuana, P. M. Blanco, M. Nedyalkova, J. L. Garcés F. Mas

Onzena Trobada de Joves Investigadors dels Països Catalans
Vilanova i la Geltrú (Spain) 27-28 January 2020

Unravelling the molecular mechanism of CO_2 hydrogenation on Ni(111): reverse water gas shift versus Sabatier reaction
P. Lozano, H. Prats, P. Gamallo, F. Illas, R. Sayós

Efecte del pH en l'estudi conformacional de les proteïnes intrínsicament desestructurades
C. Privat, S. Madurga, F. Mas, J. Rubio

Analysis of supramolecular structure of helicobacter pylori urease extracellular at different pHs by molecular dynamics simulation
S. Madurga, H. L. Barazorda-Ccahuana, P. M. Blanco, M. Nedyalkova, J. L. Garcés F. Mas

Overcoming Mott insulation by means of external mechanical compression in tam-based corfs
R. Santiago

III International Workshop on Chemistry of Group 11 Elements
Caparica (Portugal) 30-31 January 2020

Degradation of silver(I) compounds with N-heterocyclic carbenes into saline water (oral communication)
A. Cebrián, G. Aullón

The SPIRITS International Symposium
Kyoto (Japan) 6 February 2020

Shaping self-assembled mesoscale (bio)materials with microengineering (invited talk)
J. Puigmartí-Luis

International Conference on Computational Materials Science for Nanoscale Modelling – COST Action CA18234
Naples (Italy) 11-13 February 2020

Structural and Electronic Properties of Realistic TiO_2 Nanoparticles (oral communication).
Á. Morales-García

Structural and electronic structure methods and models for water splitting with nanocrystals: where we are and where we go (oral communication)
F. Illas

Modelling nanocomposite materials for catalysis: from ceria to bimetallic crystallites (invited talk)
K. M. Neyman

Symposium on Size Selected Clusters (S3C)
Davos (Switzerland) 23 February 2020

How hot are clusters in experiment? Insights from modelling finite temperature infrared spectras (invited talk)
S. T. Bromley

13th European School on Molecular Nanoscience (ESMolNa)
online (Spain) 3-5 June 2020

Improving slow spin relaxation properties by encapsulation (invited talk)
E. Ruiz

nanoGe Online Meetup Conference
online (Spain) 9-10 June 2020

Towards affordable yet accurate computational models for CO_2 electroreduction (oral communication)
F. Calle-Vallejo

Workshop on ML potentials and long-range interactions
online (Germany) 29 June – 1 July 2020

A. Bruix (co-*organization*)
https://www.department.ch.tum.de/index.php?id=4627

International Conference "New directions for modeling nanocrystal catalysts", Meeting of the COST Action CA18234
online (Israel) 7 July 2020

DFT modelling of metal nanoparticles in catalysis (invited talk)
K. M. Neyman

23rd Conference on Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction, PRES'20
online (China) 17-21 August 2020

Solvent screening and process simulation for vanillin production from lignin (oral communication)
A. E. Plesu, J. Torralba, J. Bonet-Ruiz, J. Llorens

Cleaner process and entrainer screening for bioethanol dehydration by heterogeneous azeotropic distillation (poster)
A. E. Plesu, J. L. Pellin, J. Bonet-Ruiz, J. Llorens

71st Annual Meeting of the International Society of Electrochemistry
online (Spain) 30 August – 4 September 2020

Towards a comprehensive understanding of Pt-based electrocatalysis (oral communication)
F. Calle-Vallejo

15th Conference on Sustainable Development of Energy, Water and Environment Systems (SDEWES)
online (Germany) 1-5 September 2020

Wastewater as source of sustainable secondary raw materials (oral communication)
A. E. Plesu, J. Bonet-Ruiz, P. S. Varbanov, J. J. Klemes

AEBIN Photochemistry School 2020
online (Spain) 7-9 September 2020

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, L. Cupellini, G. D. Scholes, C. Curutchet

Electrochemistry Undercover
online (Spain) 23-24 September 2020

Kinetics of the Hydrogen Evolution Reaction on MXenes (poster)
M. López, F. Viñes, F. Calle-Vallejo, K. S. Exner, F. Illas

VI International School-Conference "Catalysis: from Science to Industry"
Tomsk (Russia) 6-10 October 2020

Session 6 "Physical-chemical fundamentals of catalysis / Industrial implementation of catalytic processes" (chairman)
K. M. Neyman

Modelling of catalytic nanomaterials using Density Functional Theory (plenary lecture)
K. M. Neyman

2nd Transnational Access Visitors Meeting (TAM)
online (Spain) 22-23 October 2020

Modulation of CO_2 adsorption on cation doped TiC (oral communication)
M. López, F. Viñes, M. Nolan, F. Illas

4th Sustainable Process Integration Laboratory Scientific Conference: Energy, Water, Emission & Waste in Industry and Cities (SPIL'20)
online (Czech Republic) 18-20 November 2020

Assessment of alkanolamines for CO_2 capture by chemical absorption (oral communication)
A. E. Plesu, A. Gonzalez, T. Peiró, J. Bonet-Ruiz, J. Llorens

III Tesimarató de Química
Barcelona (Spain) 19 November 2020

Disseny racional de materials fotoactius basats en TiO_2 per a la producció d'hidrogen (oral communication)
M. R. Poo, S. T. Bromley, Á. Morales-García

CataLight Young Scientist Symposium
online (Spain) 19 November 2020

Crystal facet engineering for tailoring photoactive TiO_2 nanoparticles (oral communication)
Á. Morales-García, A. Macià, S. T. Bromley, F. Illas

CatalysisTalks Webinar Series
online (Spain) 25 November 2020

Feasibility of MXenes to catalyze the dissociation of nitrogen (oral communication)
Á. Morales-García, D. Gouveia, F. Viñes, J.R.B. Gomes, F. Illas

First International Symposium on the DFT Modelling of Materials Relevant for Water Splitting
online (Spain) 11 Desember 2020

F. Viñes, F. Illas, K. Neyman (*organization*)

DFT modelling of structure and reducibility of cerium dioxide nanoparticles doped by zirconium (invited talk)
I. Z. Koleva, H. A. Aleksandrov, K. M. Neyman, G. N. Vayssilov

Beijing Institut of Technology (BIT)
online (China) 18 Desember 2020

Exploiting controlled reaction-diffusion conditions for materials synthesis (invited talk)
J. Puigmartí-Luis

RESEARCH STAYS IN RECOGNIZED CENTERS

Ribas, J. **Center for Computational Science and E-Systems, Japan Atomic Energy Agency, Chiba (Japan)**
UB visiting researcher invited by Dr. Motoyuki Shiga.
January 2020

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 €

Magnetically steerable wireless Nanodevices for the tarGeted delivery of therapeutIc agents in any vascular rEgion of the body (ANGIE).
J. Puigmartí-Luis, University of Barcelona
952152, 2021-2025
European Commission
Amount: 4.000.000 € from where 555.000 € to University of Barcelona

Ultra-versatile Structural PRINTing of amorphous and tuned crystalline matter on multiple substrates (SPRINT).
J. Puigmartí-Luis, University of Barcelona
801464, 2018-2022
European Commission
Amount: 2.999.997,50 € (435.375 € to ETH Zürich and now to UB)

Microfluidic Crystal Factories (μ-CrysFact): a breakthrough approach for crystal engineering.
J. Puigmartí-Luis, University of Barcelona
677020, 2016-2021
European Research Council (ERC)
Amount: 1.814.128 €

Functional 2D porous crystalline materials (2DMats).
J. Puigmartí-Luis, University of Barcelona
181988, 2019-2023
Swiss National Founds
Amount: CHF 600.000, now 300,000.00 € to University of Barcelona

New approaches to nano-engineer MOF films for electronic and biotechnology applications (M-O-Films).
J. Puigmartí-Luis, University of Barcelona
2019-2023
Nanosciences Foundation: Université Grenoble Alpes
Amount: 351.000 €

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 €

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 €

Fenòmens de no-equilibri en matèria tova: de fluids complexes a teixits cel·lulars.
F. Sagués, University of Barcelona
FIS2016-78507-C2-1-P, 2017 – 2020
Ministry of Economy and Competitiveness (MINECO)

Diseño racional de nuevos catalizadores heterogeneos, electrocatalizadores y fotocatalizadores para la produccion de energía limpia sostenible a través de la conversion de H_2.
F. Illas, F. Viñes, University of Barcelona
RTI2018-095460-B-I00/AEI/FEDER, 2019 – 2021
Ministry of Economy and Competitiveness (MINECO)
Amount: 229.900 €

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 €

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, 2018-2021
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)
Amount: 104.060 €

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 €

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 €

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

Grup de Modelització i disseny de sistemes químics radicalaris.
J. M. Bofill, University of Barcelona
2017 SGR 348, 2017-2021
University and Research Grants Management Agency (AGAUR)
Amount: 20.000 €

Grup de Bioinformàtica Integrativa.
M. Cascante, University of Barcelona
2017 SGR 1033, 2017-2021
University and Research Grants Management Agency (AGAUR)

Grup d'Estructura i Funció en Macromolècules.
C. Rovira, University of Barcelona
2017 SGR 1189, 2017-2021
University and Research Grants Management Agency (AGAUR)

Grup d'Estructura Electrònica.
S. Alvarez, University of Barcelona
2017 SGR 1289, 2017-2021
University and Research Grants Management Agency (AGAUR)
Amount: 44.480 €

Grup de Biologia Computacional i Disseny de Fàrmacs.
F. J. Luque, University of Barcelona
2017 SGR 1746, 2017-2021
University and Research Grants Management Agency (AGAUR)
Amount: 65.896 €

FRAGments training NETwork.
X. Barril, University of Barcelona
FRAGNET, 2016-2020
Innovative Training Networks (UE-ITN)
Amount: 421.930 €

Alianza de Centros Severo Ochoa y Unidades María de Maeztu.
Luis Serrano, Centro de Regulación Genómica, E. Ruiz, University of Barcelona
RED2018-102506-E, 2019-2021
Ministerio de Ciencia, Investigación y Universidades
Amount: 60.000 €

Ciencia Molecular sobre superficies: Síntesis y Funcionalidad.
José Ignacio Pascual, Nanogune, J. Echeverría, University of Barcelona
RED2018-102833-T, 2019-2021
Ministerio de Ciencia, Investigación y Universidades
Amount: 15.000 €

Theoretical study on the receptor-cannabinoid affinities and dynamics.
C. Curutchet, University of Barcelona
2018 DI 043, 2019-2021
Catalan Government (GENCAT)
Amount: 33.960 €

Ramón y Cajal Programme
Jorge Echevarría, University of Barcelona
RYC-2017-22853, 2019-2020
Ministry of Economy and Competitiveness (MINECO)
Amount: 6.000 €

Interacciones no covalentes y su explotación a escala nanoscópica.
Jorge Echeverría, University of Barcelona
PID2019-109119GA-I00, 2020-2023
Ministerio de Ciencia, Investigación y Universidades
Amount: 68.000 €

Estudio teórico y espectroscópico de moléculas orgánicas birradicalarias relevantes para la química bioorgánica y los materiales moleculares multifuncionales.
Josep Maria Bofill / Ibério de P.R. Moreira, University of Barcelona
PID2019-109518GB-I00, 2020-2022
Ministry of Economy and Competitiveness (MINECO)
Amount: 60.500,00 €

Modelado de interacciones no-covalentes y cooperatividad en pares de bases de ADN (no)naturales y en cuadruplexes de guanina.
Jordi Poater, University of Barcelona
PID2019-106830GB-I00, 2020-2023
Ministry of Economy and Competitiveness (MINECO)
Amount: 60.500,00 €

Ramón y Cajal Programme.
Jordi Ciera, University of Barcelona
RYC-2018-024692-I, 2020-2021
Ministry of Economy and Competitiveness (MINECO)
Amount: 40.000 €

Beatriu de Pinós Beca Postdoctoral Grant.
Silvia Gómez-Coca, University of Barcelona
2017 BP 00080, 2018-2020
University and Research Grants Management Agency (AGAUR)
Amount: 92.000 €

Beatriu de Pinós Postdoctoral Grant.
Albert Bruix, University of Barcelona
2018 BP 00190, 2020-2023
University and Research Grants Management Agency (AGAUR)
Amount: 144.300 €

Captura de CO_2 emitido por vehiculos basados en motores de combustión, mediante adsorción en sólidos porosos.
X. Gimenez, P. Gamallo, University of Barcelona
IDI-20190124 (310437), 2019-2021
Center for Industrial Technological Development (CDTI), Recam Laser S.L.
Amount: 146.000 €

Tubulin bynamics 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
Amount: 426.210 €

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

Reposicionament basat en lligaNd (LBRS) de un compost fenòlic amb activitat anti-amiloidogènica: Una prova de concepte?
F. J. Luque, University of Barcelona
2019LLAV00016, 2020-2021
University and Research Grants Management Agency (AGAUR)
Amount: 20.000 €

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 €

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 €

Serveis en Química Computacional.
F. J. Luque, University of Barcelona
310755, 2020
Pharmacelera
Amount: 12.000 €

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

Fortalecimiento del Magíster en Química a través de la investigación teórico-experimental en Química de Materiales.
S. Conejeros, North Catholic University, Antofagasta (Chile), P. Alemany, University of Barcelona
Concurso Nacional de Atracción de Capital Humano Avanzado del Extranjero a Chile, 2020-2021
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, 2017-2021
INDUKERN (Veterinary division)

Efficient CO_2 hydrogenation through transition metals Encapsulated on MFI zeolites.
P. Gamallo, University of Barcelona
QS-2020-1-0028, **QS-2020-2-0003**, 2020
Spanish Supercomputing Network (RES)

CO_2 conversion into light fuels activated by H/H_2 over transition metal encapsulated in MFI zeolites (TM@S-1).
P. Gamallo, University of Barcelona
QS-2020-3-0023, 2020
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, **QS-2020-2-0020**, 2019-2020
Spanish Supercomputing Network (RES)

Machine-learning adsorption energies on bimetallic surfaces.
K. Neyman, University of Barcelona
QS-2020-3-0015, **QS-2020-1-0017**, 2020-2021
Spanish Supercomputing Network (RES)

Cu- and Ni-based bimetallic nanoparticles: global optimization and propagation of exchange-correlation functional error estimates.
Albert Bruix, University of Barcelona
QS-2020-3-003, 2020-2021
Spanish Supercomputing Network (RES)

Mechanisms of mutation resistance in hemagglutinin: Is the uncleaved form HA0 the right target?
T. Ginex, F. J. Luque, CSIC, University of Barcelona
2020225437, 2020-2021
Partnership for Advanced computing in Europe (PRACE)

Targeting conformational changes implicated in early events of viral entry.
F. J. Luque, University of Barcelona
COVID-19, 2020
Partnership for Advanced computing in Europe (PRACE)

Identificacion de inhibidores de la proteasa Mpro del virus COVID-19 por reposicionamiento de medicamentos.
J. J. Pérez, Universitat Politècnica de Catalunya
COV20/00052, 2020
Instituto de Salud Carlos III (ISCA)
Amount: 14.500 €

Identificacion de inhibidores de la proteina-S del virus Covid-19 por reposicionamiento de medicamentos.
J. M. Granadino, Universidad de Jaen
CV20-43338, 2020-2021
Junta de Andalucía (JUAN)
Amount: 28.583 €

PATENT OR MARK APPLICATION

Gasoline composition comprising indoline.
J. Delgado Diestre, M. López Reyes, F. J. Luque Garriga (University of Barcelona)
20382663.1-1101

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