Institut de Química Teòrica
i Computacional

EXCELENCIA
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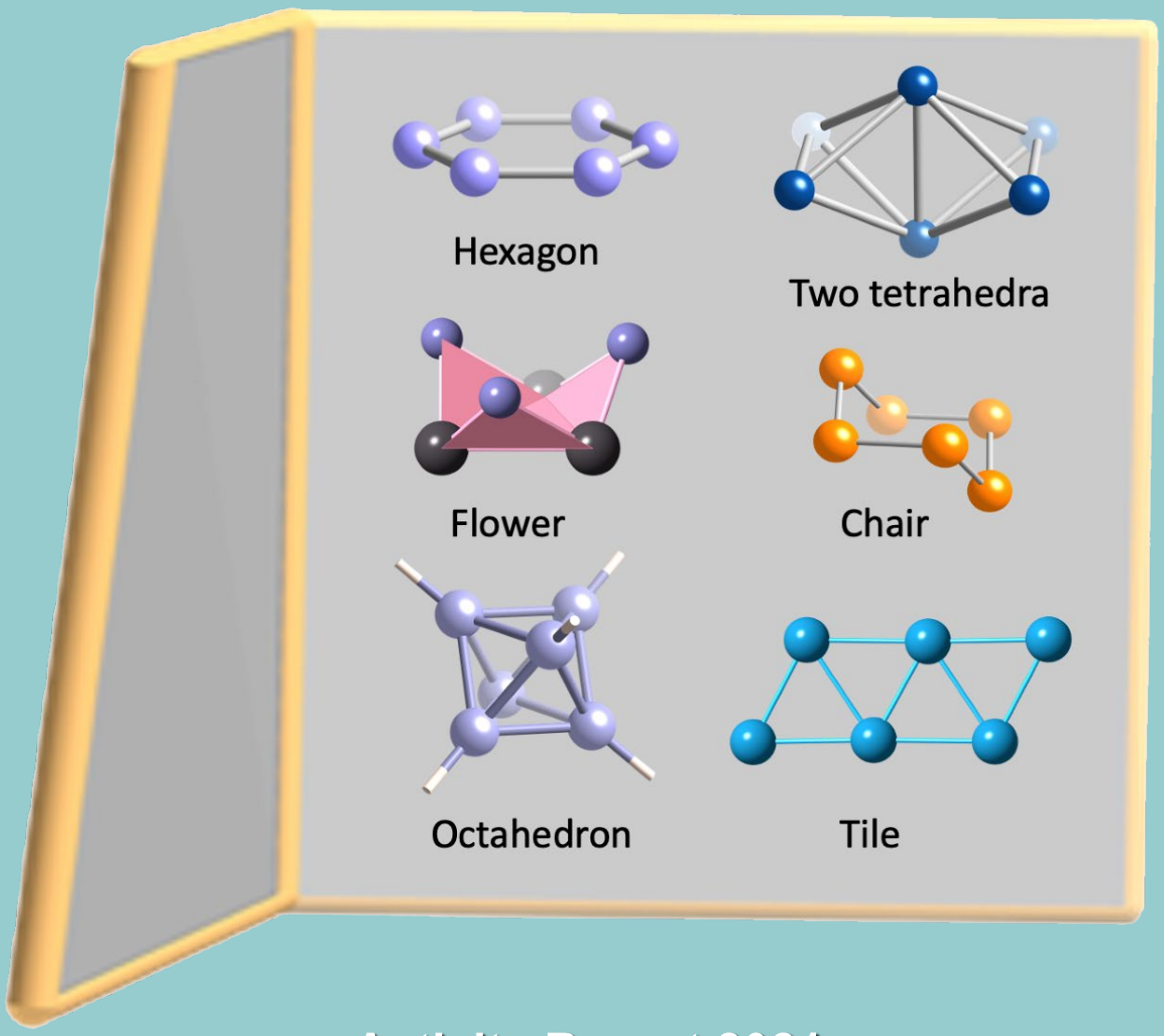
UNIVERSITAT DE
BARCELONA

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



Activity Report 2021

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 an ordinary session on November 21st, 2007. From April 2018 I have the honor to serve as Director and I want to take the opportunity of being at the forefront of the IQTCUB's annual. Additionally, from the point of view of external recognition, the María de Maeztu awarding has allowed to incorporate new grant holders and postdocs into the Institute giving us an increase in the quality and quantity of our research. Another important point has been the incorporation of senior researchers through programs like Beatriu de Pinós, Juan de la Cierva, Junior Group Leader La Caixa, Ramón y Cajal and ICREA.

The common goal of the research projects developed at the Institute is the use of quantum chemistry methods, although recently with the inclusion of experimental groups from our departments, new collaborations beyond Computational Chemistry have been initiated fostering and increasing the multidisciplinary character of our research. Traditionally, IQTC research is different from what everyone expects from a traditional chemist since the instrumentation used by our researchers is not located in a traditional laboratory but in a computational "laboratory" that is usually the gateway to our resources or to supercomputing centers with even greater computational capacity.

Computational chemistry is in a period of profound change. Due to the availability in the short/medium term of quantum computers that will completely change our usual way of working. Within quantum computing, developing new computational methods that can take advantage of this new type of computers is crucial at this time. Thus, in 4-5 years' time, when computers with thousands of qubits will be available, it will be possible to study highly complex systems with a precision that is not possible with classical computers. This will represent an additional step forward in the studies that are currently being carried out. According to this, this field will provide new concepts that will allow progress in different aspects such as the rational design of new materials with specific physical properties and their application in electronics and magnetic devices; in the discovery of new drugs and in the understanding of the biochemical processes behind them; in new reactions that improve chemical processes to make them more efficient and environmentally friendly; and in the proposal of new sustainable energy sources to overcome the challenges facing our society today.

Eliseo Ruiz
Director of IQTCUB

Institut de Química Teòrica i Computacional

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 2021 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 121 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
Álvarez 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
Reigada Sanz	Ramón	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
Ribas Ariño	Jordi	SPAIN (M)	Materials Science & Physical Chemistry
Viñes Solana	Francesc	SPAIN (M)	Materials Science & Physical Chemistry

ICREA Research Professors

Barril	Xavier	SPAIN (M)	Pharm. & Pharm. Tech. & Phys. Chem.
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 (M)	Inorganic Chemistry & Organic Chemistry

Other Categories (Professors Lectors)

Estarellas	Carolina	SPAIN (F)	Nutrition, Food Sciences & Gastronomy
Gómez Coca	Silvia	SPAIN (F)	Inorganic Chemistry & Organic Chemistry
Jover Modrego	Jesús	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
Juárez Jiménez	Jordi	SPAIN (M)	Pharm. & Pharm. Tech. & Phys. Chem.
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

Aragonès	Albert	SPAIN (M)	Materials Science & Physical Chemistry
Bruix Fusté	Albert	SPAIN (M)	Materials Science & Physical Chemistry
Fumanal Quintana	Maria	SPAIN (M)	Materials Science & Physical 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
Vela Llausi	Sergi	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
Guix Noguera	Maria	SPAIN (F)	Materials Science & Physical Chemistry

Contracte Projecte de Recerca

Alonso Benito	Gerard	SPAIN (M)	Materials Science & Physical Chemistry
Belce	Yonca	TURKEY (F)	Materials Science & Physical Chemistry
Mattera	Michele	ITALY (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
Macià Escatllar	Antoni	SPAIN (M)	Materials Science & Physical Chemistry
Nin Hill	Alba	SPAIN (F)	Inorganic Chemistry & Organic 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)	Química Inorgànica i Química Orgànica
Vílchez Pérez	David	SPAIN (M)	Nutrition, Food Sciences & Gastronomy

FI Grant (Catalan Government Program)

Aledavood	Elnaz	SPAIN (F)	Nutrition, Food Sciences & Gastronomy
Mariñoso Guiu	Joan	SPAIN (M)	Materials Science & Physical Chemistry
Martín Rodríguez	Alejandro	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
Ozaydin	Gül Beste	TURKEY (F)	Pharm. & Pharm. Tech. & Phys. Chem.
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
Castro Latorre	Pablo	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
Farris	Riccardo	ITALY (F)	Materials Science & Physical 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
Romeo	Eleonora	ITALY (F)	Materials Science & Physical 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

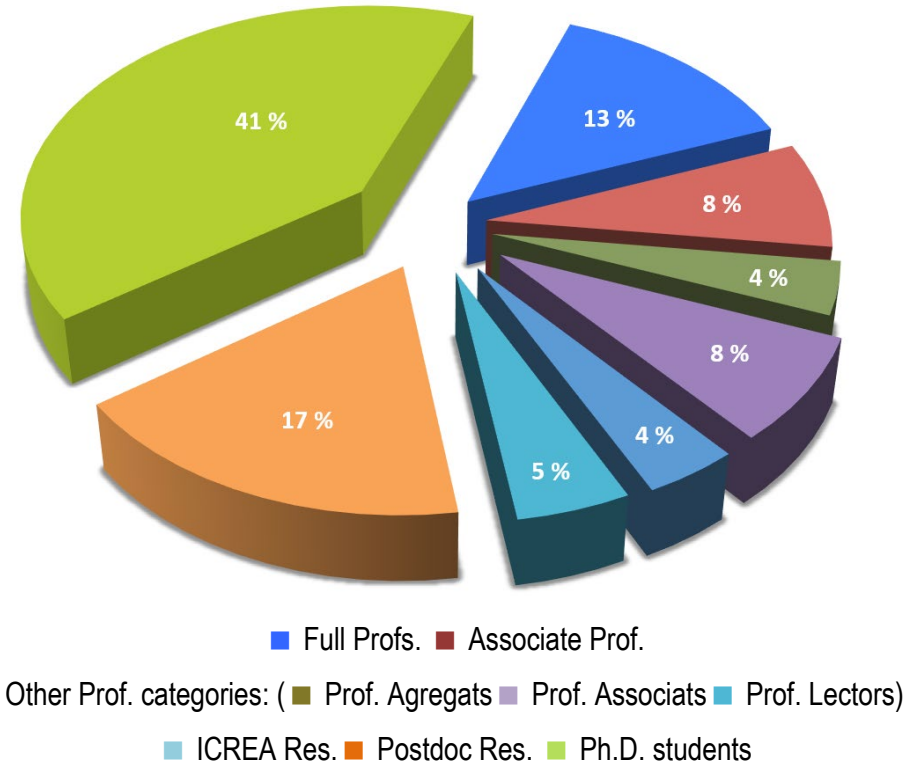
Dias da Cunha	Renato	BRAZIL (M)	Pharm. & Pharm. Tech. & Phys. Chem.
López Berbel	Martí	SPAIN (M)	Materials Science & Physical Chemistry
Gonzalo Palao	Daniel	SPAIN (M)	Pharm. & Pharm. Tech. & Phys. Chem.
Navarro Maestro	Laia	SPAIN (F)	Inorganic Chemistry & Organic Chemistry
Roncero Barrero	Cristina	SPAIN (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

Campos-Vicens	Lluis	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
De Oliveira Almeida	Michell	BRASIL (M)	Materials Science & Physical Chemistry
Figueras Valls	Marc	SPAIN (M)	Materials Science & Physical Chemistry
García Gonzalo	Lluc	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
Gil	Diego	ARGENTINA (M)	Inorganic Chemistry & Organic Chemistry
Meng	Ling	CHINA (M)	Materials Science & Physical Chemistry
Nicholas	James	UK (M)	Materials Science & Physical Chemistry
Quinlivan Domínguez	Jon Eunan	SPAIN (M)	Materials Science & Physical Chemistry
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 each.

CALCULATION CLUSTERS

cerqt2 (*invested value 100.000 €*)

Machine type	SUN cluster (1 rack)
Operating system	SLES10
Services	*Calculation cluster and disk server (raid of 2.5TB)*. Internal DHCP server
Structure	Master + 45 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)

45 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)

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 340.000 €*)

Machine type	Gigabyte Cluster
Operating System	Centos 7.2
Services	Calculation cluster
Structure	30 nodes
Notes	64 bits processors

Specifications

26 Gigabyte R13
CPU: 2 x 2,9 GHz AMD EPYC 7542 32-core processor (64 cores)
RAM: 1 TB
HD: 1 x 2 TB SATA hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (internal administration network) + 2 x 10 GB network card

4 Gigabyte R182
CPU: 2 x 2,3 GHz AMD EPYC 7642 48-core processor (96 cores)
RAM: 1 TB
HD: 1 x 2 TB SATA hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (internal administration network) + 2 x 10 GB network card

Iqtc10 (*invested value 100.000 €*)

Machine type	Gigabyte Cluster
Operating System	Centos 7.2
Services	Calculation cluster
Structure	5 nodes (20 GPU RTX 3090)
Notes	64 bits processors

Specifications

5 Gigabyte G482-Z54-00
CPU: 2 x 3,0 GHz AMD EPYC 7313 16-core processor (32 cores)
RAM: 128 GB
HD: 1 x 2 TB SATA hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (internal administration network) + 2 x 10 GB network card
GPU: 4 x RTX3090 NVIDIA

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 64.000 €*)

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

Machine type	Supermicro
Operating system	Ubuntu Server 20.04
Services	Storage service cluster with 80TB 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: 4 x 2,40 GHz Xeon Silver 4314 (64 cores)
RAM: 128 GB
HD: 8 x 10 TB (raid 5)
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. 1 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.....5,092 c

Memory.....67,566 GB RAM

Calculation disk capacity .....221 TB

Data user disk capacity.....75 TB

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

*2.260.000 €**

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

II. IQTCUB ACTIVITIES

II.1 GENERAL ACTIVITIES (COURSES, GRANTS AND DISSEMINATION)

Next, a description of activities and actions promoted by IQTCUB through 2021 is provided.

a. ***Promotion and Encouragement of Research.*** This year the IQTCUB has offered one postmaster and two Master+UB fellowships to help students to initiate a scientific career. At this time, MSc. Eloi Sánchez has joined the postmaster fellowship and Mr. Christian Domínguez and Mr. Miquel Alles have joined the Master+UB fellows.

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

b. ***IQTC Women.*** A new section started where all IQTC's female scientists expose briefly her research and related activities. In 2021 have participated Carme Rovira, Alba Nin-Hill, Mercè Deumal, Beste Ozaydin, Silvia Gómez, Lorena Vega, Mª Nuria Peralta, Laia Navarro, Salomé Llabrés, Beatriz Piniello, Irene Cuxart, Carme Sousa and Anabel Jurado.

Panel promoting the IQTC women research.

c. ***Scientific Dissemination Activities.*** The following scientific dissemination activities have been performed during 2021:

1. Carme Rovira, "El glaseado que camufla el virus". El Pais - 18/Jan/21, https://elpais.com/ciencia/2021-01-18/el-glaseado-que-camufla-al-coronavirus.html
2. Xavier Giménez, "Pandèmia i Paràsits". Setmanari Montbui Journal 1924, Jul/21.
3. Xavier Giménez: 20 talks at "UB s'Apropa", 10 Talks "Gaudir UB", 10 Talks "Seminaris Casa Elizalde; 2 Talks at Toc–Toc UB Science Dissemination; 1 Talk at Science–Week, FCRi; 1 Welcome Speech at Facultat de Química, UB; 13 Interviews in Media (Press, Radio, TV).

4. Josep Puigmartí, Media interview at Exterior.cat – 19/Jul/21, https://exterior.cat/a-fons/josep-puigmarti-hi-ha-molts-professionals-a-les-universitats-que-no-tenen-possibilitat-dinvestigar/

Other dissemination activities carried out for IQTC members during 2021 are the following:

1. *"Fem Química al Laboratori"*
   Antonio Aguilar, Carme Sousa i Pablo Gamallo, January-February 2021.
2. *"VII Festa de la Ciència de la UB"*
   Pablo Gamallo, University of Barcelona, 25-28 May 2021.
   http://www.ub.edu/laubdivulga/festacienciaub/festacienciaVII/index.html

d. ***IQTCUB Virtual Workshop.*** This one-day workshop aimed at the dissemination of the research done at the IQTCUB took place on Feb 29th, 2021 at it was organized by Dr. Jordi Cirera. The IQTCUB members and internationally acknowledged speakers present the most recent work. This year we highlight the participation of Prof. Dr. Xiaobo Sun from the Amsterdam Center for Multiscale Modeling with the invited lecture entitled Rational design of Iron-based catalysts for cross-coupling reactions; Sr. Daniel Vidal that presented the talk entitled *DFT benchmarking of spin-crossover phenomena in mononuclear Fe(III)-systems*; Dr. Federico Calle from the Department of Materials Science and Physical Chemistry of the University of Barcelona that presented the talk entitled *Toward more accurate and affordable computational models for CO_2 electroreduction*; Dr. Salomé Llabrés from the Department of Nutrition, Food Sciences and Gastronomy of the University of Barcelona that presented *MacA: a molecular valve within the MacABTolC efflux pump*; Dr. Albert Bruix from the Department of Materials Science and Physical Chemistry of the University of Barcelona that presented the talk entitled *Addressing the complexity of nanostructured materials in catalysis modelling* and finally, Prof. Mercè Deumal from the Department of Inorganic and Organic Chemistry of University of Barcelona that talk about *Different mechanisms of stabilization of regular p-stacks of radicals in switchable dithiazolyl-based materials*.

e. ***Summer Computational School (X edition).*** From June 28th to July 2nd Prof. Gabriel Aullón have organized the summer computational school entitled *Computational Modelling: from Molecules to Materials*. In this edition, the sessions were given by the following researchers:

-Linux (J. Inglés and I. Zamorano)

-Enllaç i Estructura (G. Aullón and S. Gómez)

-Dinàmica Molecular (M. González and P. Gamallo)

-Reactivitat Molecular (J. Jover and J. Cirera)

-Estats Excitats (M. Deumal)

-Teoria de Bandes (E. Ruiz)

-Propietats de Materials (S. Bromley)

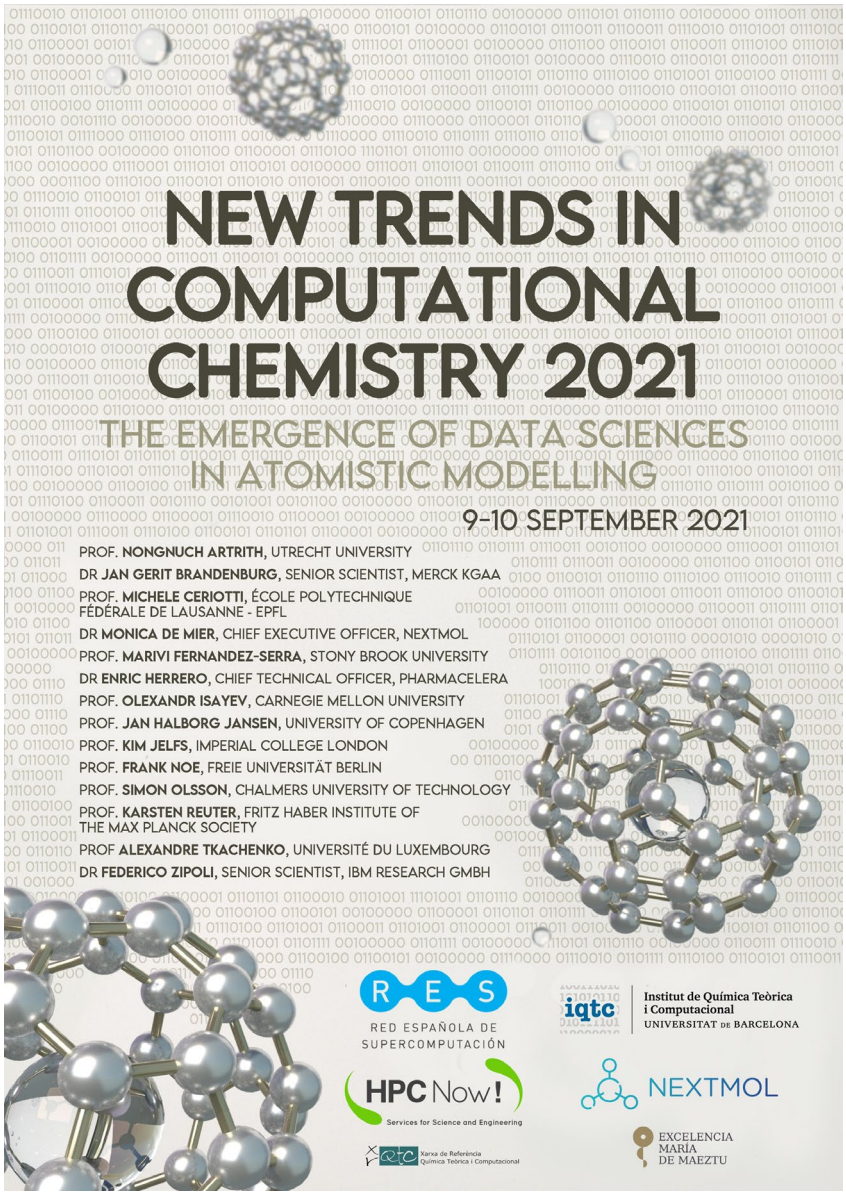
-Catàlisi Heterogènia (F. Calle)

-Superfícies i Defectes (A. Morales)

-Machine Learning (A. Bruix)

Some students following the course.

f. ***New Trends in Computational Chemistry.*** This workshop was held virtually on September 9th and 10th and it brought together experts in the application and development of Data Science methods applied to atomistic modelling, providing an overview of recent advances, state of the art approaches, and future perspectives. It consisted of two days of talks by invited speakers from both academia and industry.



Panel promoting the New Trends workshop.

II.2 IQTCUB SEMINARS AND CONFERENCES

During 2021 IQTC has organized the following seminars and conferences:

1. **Dr. Stefan Grimme** (Mulliken Center for Theoretical Chemistry, University of Bonn), Bonn, Germany.
   Low-cost quantum chemistry methods
   1 July 2021.

2. **Dr. Roser Valentí** (Institut für Theoretische Physik, Goethe-Universität Frankfurt) Frankfurt, Germany.
   Quantum materials design: challenges and opportunities
   27 May 2021.

3. **Dr. Benedetta Mennucci** (Dipartimento di Chimica e Chimica Industriale, Università di Pisa), Pisa, Italy.
   Proteins and light: a multiscale problem in space and time
   15 April 2021.

II.3 IQTCUB INVITED RESEARCHERS

During 2021, a total of nine researchers have spent some time at the IQTCUB collaborating in different research projects.

1. **Ling Meng** (HPC3 Europa visitor).
   South China Normal University, China.
   April-July 2021.

2. **Laia Delgado** (HPC3 Europa visitor).
   University of Cambridge, UK.
   May-August 2021.

3. **Elizabeth Sargeant** (HPC3 Europa visitor).
   University of Birmingham, UK.
   October 2021 - January 2021.

4. **Michell de Oliveira Almeida** (invited researcher)
   Universidade de Sao Paolo, Brazil.
   August-September 2021.

5. **Piero Ferrari** (HPC3 Europa visitor).
   Radboud University, Netherlands.
   May-July 2021.

6. **Brigida Piergiovanni** (Erasmus).
   University of Bari, Italy.
   April-September 2021.

7. **Katerina Barmpidi** (Erasmus + HPC3 Europa visitor).
   University of Athens, Greece.
   March-August 2021.

8. **Riccardo Farris** (HPC3 Europa visitor).
   University of Cagliari, Italy.
   January-April 2021.

9. **Diego M. Gil** (invited researcher).
   University of Tucumán, Argentina.
   May 2021 - January 2022.

III. SCIENTIFIC ACTIVITY OF IQTCUB MEMBERS

III.1 HIGHLIGHTS FROM MOST RELEVANT RESULTS

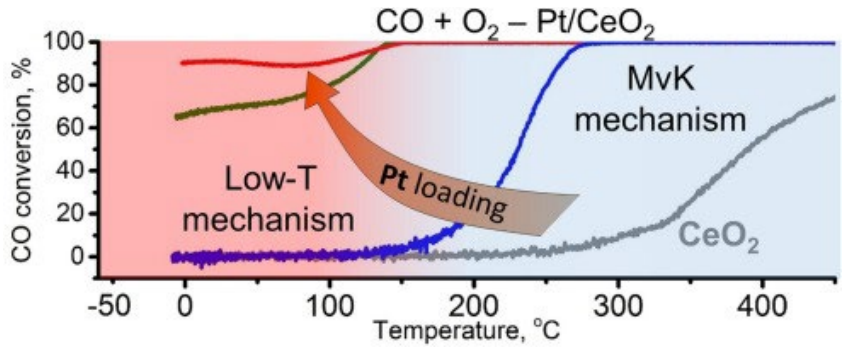
Here some of the most relevant results corresponding to every IQTCUB main research line are presented.

LINE 1. CLEAN AND SUSTAINABLE ENERGY

CO oxidation activity of Pt/CeO_2 catalysts below 0°C: platinum loading effects.

A. I. Boronin, E. M. Slavinskaya, A. Figueroba, A. I. Stadnichenko, T. Y. Kardash, O. A. Stonkus, E. A. Fedorova, V. V. Muravev, V. A. Svetlichnyi, A. Bruix, K. M. Neyman.

Appl. Catal. B: Environ. *286* (2021) 119931.

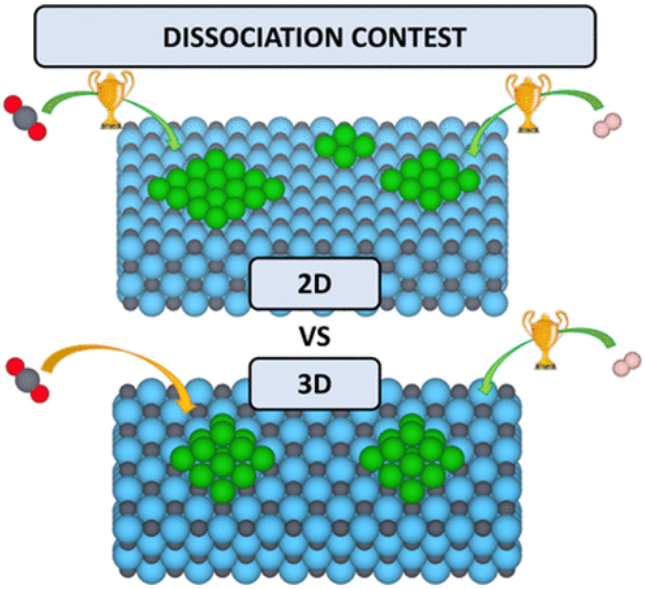


Reducing the operating temperature of oxidation catalysts is important for designing energy efficient processes, extending catalyst lifetime, and abating pollutants, especially in cold climates. Herein, high CO oxidation activity at sub-ambient temperatures is reported for Pt/CeO_2 catalysts with high content of Pt in the form of dispersed Pt^{2+} and Pt^{4+} centres. Whereas the reference 1 wt% Pt catalyst was active for CO oxidation only above 100°C, the 8 and 20 wt% Pt catalysts converted 60 and 90 % of CO, respectively, below 0°C. Ionic platinum was shown to facilitate oxygen release from ceria and lower the light-off temperature of the reaction occurring through the Mars-van-Krevelen mechanism. However, the remarkable activity observed at sub-ambient temperatures for the ≥8 wt% Pt catalysts is proposed to involve O_2 and CO reactants weakly adsorbed on PtO_x clusters. The synergies between ionic platinum and nanostructured ceria reported in this work advance the knowledge-driven design of catalysts for low-temperature oxidation reactions.

Assessing the activity of Ni clusters supported on TiC(001) toward CO_2 and H_2 dissociation.

P. Lozano-Reis, H. Prats, R. Sayós, J. A. Rodriguez, F. Illas.

J. Phys. Chem. C *125* (2021) 12019-12027.

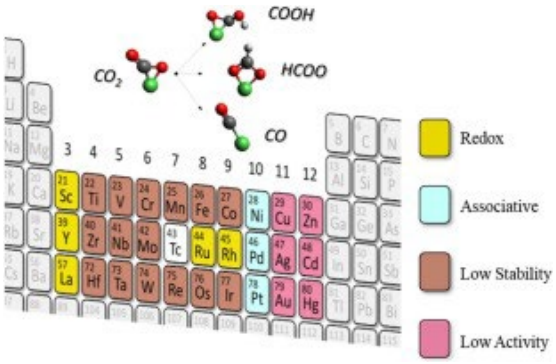


Small Ni particles supported on TiC(001) were shown to display a very high activity for the catalytic hydrogenation of CO_2 but the underlying chemistry is, to a large extent, unknown. Here, by means of periodic density functional theory (DFT) calculations with the BEEF–vdW functional, we explore the adsorption and subsequent dissociation of CO_2 and H_2 on several Ni_n clusters (n = 4, 9, 13, and 16) supported on TiC(001) and compare the results to those obtained for the bare Ni(111) and TiC(001) surfaces using exactly the same computational approach. The calculations reveal that the Ni_n/TiC system exhibits stronger adsorption energies and lower dissociation energy barriers for CO_2 and H_2 than the bare Ni(111) and TiC(001) surfaces. This is in line with the experimental finding evidencing that the Ni/TiC system has a catalytic activity higher than that of the separated Ni and TiC constituents. In addition, the calculated results show that two-dimensional (2D) supported clusters adsorb CO_2 and H_2 stronger than the three-dimensional (3D) supported clusters and also the 2D clusters exhibit lower energy barriers for CO_2 dissociation. Within the 2D supported clusters, larger particles feature slightly stronger adsorption energies and lower CO_2 dissociation energy barriers. Finally, H_2 dissociation proceeds with a very low energy barrier on all of the studied models, which makes these novel systems potential good candidates for hydrogenation reactions.

Zeolite-encapsulated single-atom catalysts for efficient CO_2 conversion.

G. Alonso, E. López, F. Huarte-Larrañaga, R. Sayós, H. Prats, P. Gamallo.

J. CO2 Util. *54* (2021) 101777.

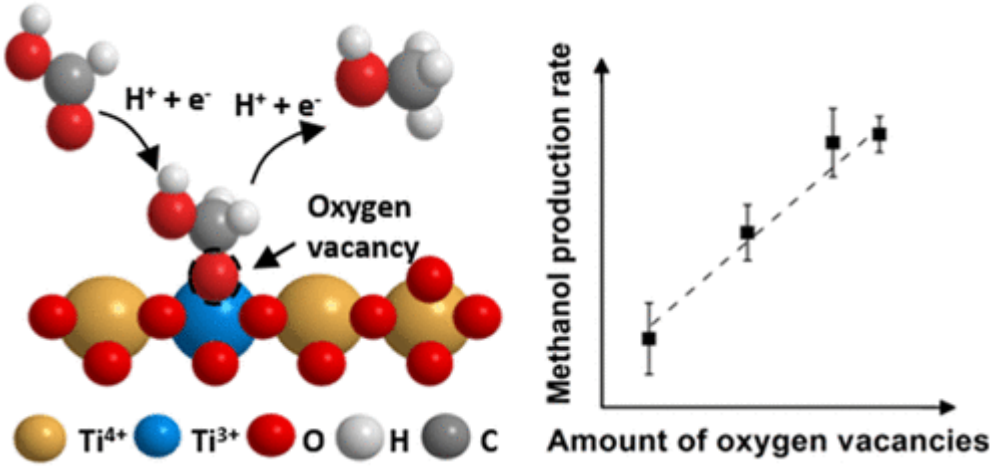


Zeolite-supported single-atom catalysts (SACs) have emerged as a novel class of cheap and tuneable catalysts that can exhibit high activity, selectivity and stability. In this work, we conduct an extensive screening by means of density functional theory calculations to determine the usefulness of 3d, 4d and 5d transition metal (TM) SACs-supported in MFI-type Silicalite-1 zeolite for CO_2 conversion. Two reaction mechanisms are considered, namely the redox direct CO_2 dissociation and associative hydrogen-assisted CO_2 dissociation mechanisms. Early TM SACs exhibit the lowest energy barriers, which follow the redox mechanism. These energy barriers raise when going right in the periodic table up to group 10, where they become prohibitive and the associative mechanism should dominate. By also considering their resistance to aggregation, we support the use of Sc, Y, La, Ru, Rh, Ni, Pd and Pt as potentially active and stable catalysts for CO_2 conversion, given their low energy barriers and strong interaction with the zeolite framework.

Toward efficient tandem electroreduction of CO_2 to methanol using anodized titanium.

W. J. Teh, O. Piqué, Q. H. Low, W. Zhu, F. Calle-Vallejo, B. S. Yeo.

ACS Catal. *11* (2021) 8467-8475.

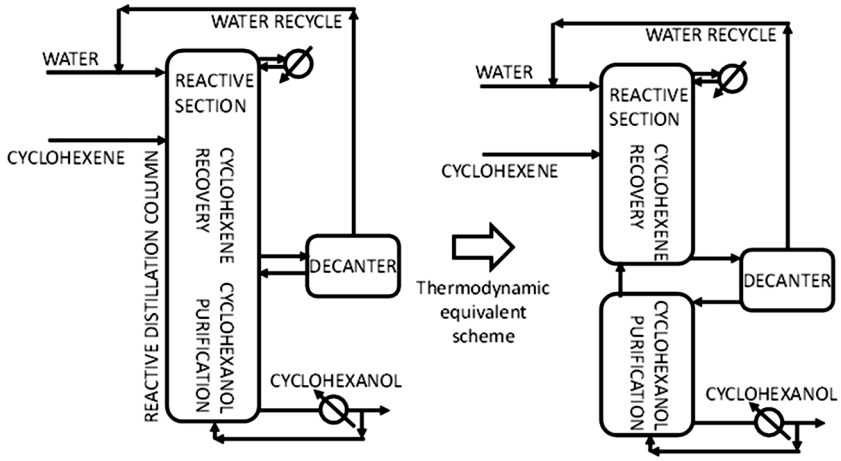


The electroreduction of CO_2 (CO_2RR) using renewable electricity is an appealing route to synthesize methanol (CH_3OH), a valuable C_1 feedstock and fuel. Unfortunately, there are still no workhorse electrocatalysts with suitable activity and selectivity for this reaction. Currently, formic acid (HCOOH), CO, and methane are the most common C_1 products. Since multielectron electrocatalytic reactions can be severely affected by adsorption-energy scaling relations, a tandem process likely offers a higher efficiency. Therefore, we strategized to reduce CO_2 to HCOOH and then reduce HCOOH to CH_3OH. While the former step can be accomplished with ease using post-transition metals, the latter is extremely difficult due to the electrochemical inertness of HCOOH. Herein, we develop anodized titanium catalysts containing Ti^{3+} sites and oxygen vacancies (termed as TOVs), which can reduce HCOOH to CH_3OH with a remarkable Faradaic efficiency of 12.6% and a partial current density of −2 mA/cm^2 at −1.0 V versus reversible hydrogen electrode (RHE). Using electron paramagnetic resonance spectroscopy and cyclic voltammetry, we show that the population of TOVs on the catalyst is positively correlated with the production of CH_3OH. Density functional theory (DFT) calculations identify TOVs at defects as the active sites in a vacancy-filling pathway mediated by $*H_2COOH$. We further provide holistic screening guidelines based on the *HCOOH and $*H_2COOH$ binding energies alongside TOV formation energies. These can open the path for the high-throughput automated design of catalysts for CH_3OH synthesis from tandem CO_2 electrolysis.

Greenhouse gas emissions reduction by process intensification: Reactive distillation column with side decanter.

A. E. P. Popescu, J. Bonet, J. Llorens.

Energy Environ. *32* (2021) 1457-1478.

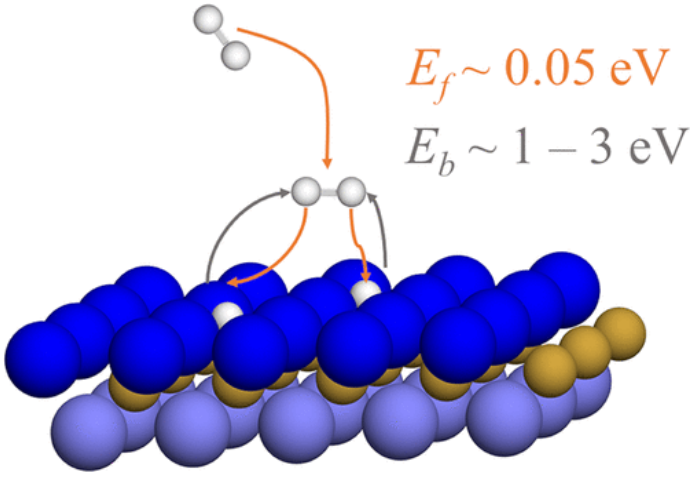


Direct hydration of cyclohexene to produce cyclohexanol is the industrial process with a lower raw material cost but with a quite expensive process. Large energy consumption is consequence of large cyclohexene recycle related with its unfavourable chemical equilibrium. This study corroborates that the Asahi process is a good candidate for intensification avoiding the cyclohexene recycle. Rigorous simulation shows that a single reactive distillation column, with a side decanter, operated at total reflux, allows overcoming the chemical equilibrium limitations as the product is continuously collected by the column bottoms and the heat of reaction is directly used to separate the product by distillation. The novel process is studied and compared to the classical Asahi process. An energy comparison with the available processes proposed in the literature is performed. Therefore, achieving more energy-efficient processes leads to lowering their environmental impact, thus decreasing the carbon dioxide emissions. Applying the proposed methodology for cyclohexanol production, more than 67,000 t CO_2/y emissions can be avoided compared to the nowadays used classical process, thus the potential savings applying process intensification to the chemical industry are very large and worth further investigation.

Thermodynamics and kinetics of molecular hydrogen adsorption and dissociation on MXenes: relevance to heterogeneously catalyzed hydrogenation reactions.

M. López, A. Morales-García, F. Viñes, F. Illas.

ACS Catal. *11* (2021) 12850-12857.

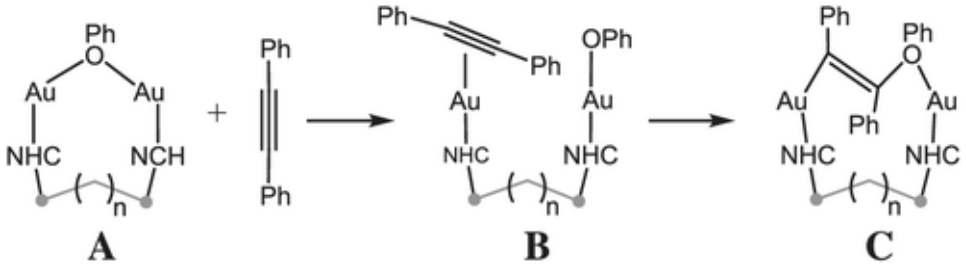


The interaction of molecular hydrogen with a series of 28 two-dimensional (2D) carbides and nitrides, known as MXenes, has been studied by means of periodic density functional calculations. This study shows that trends in atomic and molecular adsorption energies can be rationalized in terms of the electrostatic potential above the surface site and the Bader charge on the surface metal atoms. For all systems, molecular hydrogen is found to dissociate with almost negligible barriers, meaning that at low temperature the MXene surface will be passivated by adsorbed atomic hydrogen. The conditions at which the MXene surface is partly covered and, hence, able to participate in hydrogenation reactions are investigated by means of ab initio thermodynamics and phase diagrams derived from microkinetic simulations. The first provide the equilibrium conditions for a given H coverage on the MXene of interest, whereas the second provides the conditions at which a given configuration is reachable at the working conditions. For fast enough processes, both approaches necessarily lead to the same result, but this may differ when high energy barriers are involved, as it the case here for the H adatoms recombination step. With this suite, we show that Fe_2C, W_2N, and Mo_2C are promising hydrogenation catalysts. This work serves as a first step toward the rational design and implementation of MXene-based hydrogenation catalysts.

Chelation enforcing a dual gold configuration in the catalytic hydroxyphenoxylation of alkynes.

S. Escayola, J. Poater, M. Ramos, J. A. Luque-Urrutia, J. Duran, S. Simon, M. Solà, L. Cavallo, S. P. Nolan, A. Poater.

Appl. Organomet. Chem. *35* (2021) e6362.



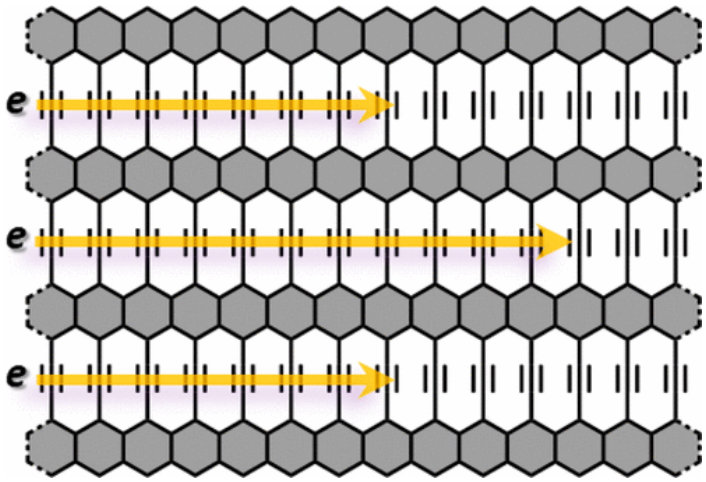
The functionalization of alkynes by Au (N-heterocyclic carbene, NHC) complexes via the hydrophenoxylation reaction is a paradigm for the discussion between mono and dual metal catalysis. With the aim of mimicking the framework containing two gold units, achieved with molecular boxes, two NHC ligands were joined here with a chelated chain and this motif was examined in the hydrophenoxylation/hydroalkoxylation reactions through DFT calculations. This synthetic motif transforms the standard hydrophenoxylation intermolecular reaction from an inter- into an intra-molecular nucleophilic attack, when forming the C–O bond. Various chain lengths were tested with regard to the coordination of the alkyne to the cationic NHC-gold(I) centre.

LINE 2. NANOMATERIALS AND NANOELECTRONICS

Acetylene-mediated electron transport in nanostructured graphene and hexagonal boron nitride.

I. Alcón, N. Papior, G. Calogero, F. Viñes, P. Gamallo, M. Brandbyge.

J. Phys. Chem. Lett. *12* (2021) 11220-11227.

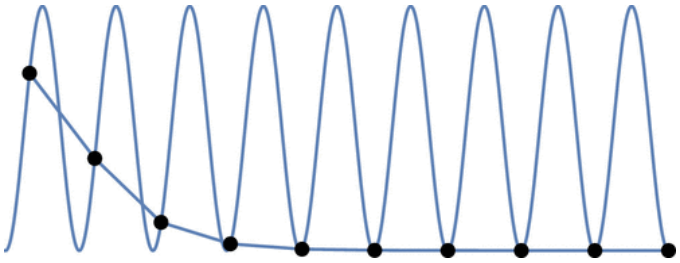


The discovery of graphene has catalyzed the search for other 2D carbon allotropes, such as graphynes, graphdiynes, and 2D π-conjugated polymers, which have been theoretically predicted or experimentally synthesized during the past decade. These materials exhibit a conductive nature bound to their π-conjugated sp^2 electronic system. Some cases include sp-hybridized moieties in their nanostructure, such as acetylenes in graphynes; however, these act merely as electronic couplers between the conducting π-orbitals of sp^2 centers. Herein, via first-principles calculations and quantum transport simulations, we demonstrate the existence of an acetylene-meditated transport mechanism entirely hosted by sp-hybridized orbitals. For that we propose a series of nanostructured 2D materials featuring linear arrangements of closely packed acetylene units which function as sp-nanowires. Because of the very distinct nature of this unique transport mechanism, it appears to be highly complementary with π-conjugation, thus potentially becoming a key tool for future carbon nanoelectronics.

Barnes update applied in the Gauss-Newton method: an improved algorithm to locate bond breaking points.

J. M. Bofill, R. Valero, J. Ribas-Ariño, W. Quapp.

J. Chem. Theory Comput. *17* (2021) 996-1007.

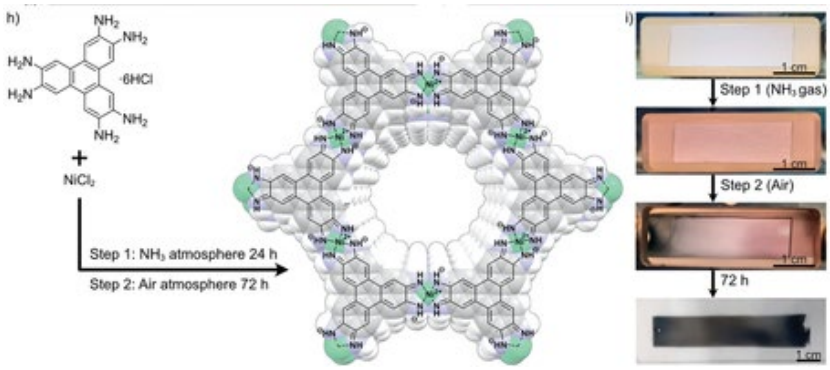


A mechanochemical reaction is a reaction induced by mechanical energy. A general accepted model for this type of reaction consists of a first-order perturbation on the associated potential energy surface (PES) of the unperturbed molecular system due to mechanical stress or pulling force. Within this theoretical framework, the so-called optimal barrier breakdown points or optimal bond breaking points (BBPs) are critical points of the unperturbed PES where the Hessian matrix has a zero eigenvector that coincides with the gradient vector. Optimal BBPs are “catastrophe points” that are particularly important because their associated gradient indicates how to optimally harness tensile forces to induce reactions by transforming a chemical reaction into a barrierless process. Building on a previous method based on a nonlinear least-squares minimization to locate BBPs, we propose a new algorithm to locate BBPs of any molecular system based on the Gauss–Newton method combined with the Barnes update for a nonsymmetric Jacobian matrix, which is shown to be more appropriate than the Broyden update. The efficiency of the new method is demonstrated for a multidimensional model PES and two medium size molecular systems of interest in enzymatic catalysis and mechanochemistry.

Synthesis of 2D porous crystalline materials in simulated microgravity.

N. Contreras-Pereda, D. Rodríguez-San-Miguel, C. Franco, S. Sevim, J. P. Vale, E. Solano, W. -K. Fong, A. Del Giudice, L. Galantini, R. Pfattner, S. Pané, T. S. Mayor, D. Ruiz-Molina, J. Puigmartí-Luis.

Adv. Mater. *33* (2021) 2101777

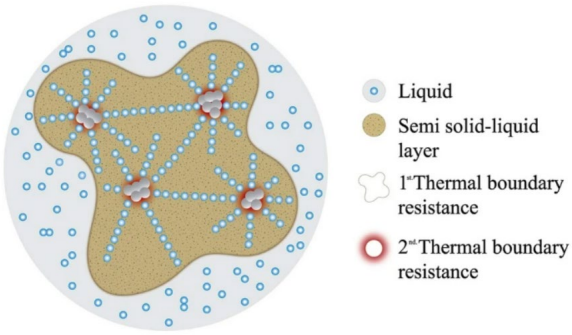


To date, crystallization studies conducted in space laboratories, which are prohibitively costly and unsuitable to most research laboratories, have shown the valuable effects of microgravity during crystal growth and morphogenesis. Herein, an easy and highly efficient method is shown to achieve space-like experimentation conditions on Earth employing custom-made microfluidic devices to fabricate 2D porous crystalline molecular frameworks. It is confirmed that experimentation under these simulated microgravity conditions has unprecedented effects on the orientation, compactness and crack-free generation of 2D porous crystalline molecular frameworks as well as in their integration and crystal morphogenesis. It is believed that this work will provide a new “playground” to chemists, physicists, and materials scientists that desire to process unprecedented 2D functional materials and devices.

Understanding the abnormal thermal behavior of nanofluids through infrared thermography and thermo-physical characterization.

A. Svobodova-Sedlackova, A. Calderón, C. Barreneche, P. Gamallo, A. I. Fernández.

Sci. Rep. *11* (2021) 4879.

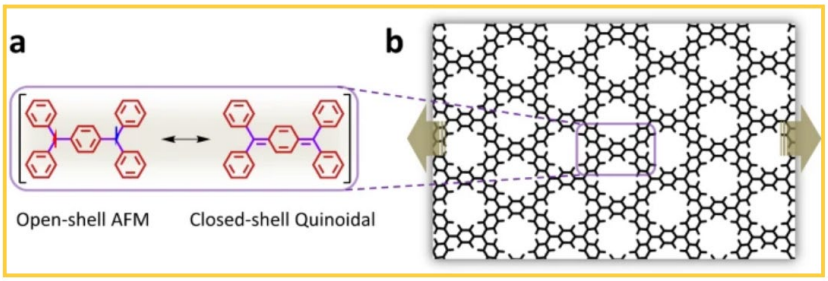


Nanofluids (NFs) are colloidal suspensions of nanoparticles (NPs) within a base fluid. Unlike conventional mixtures, NFs exhibit dramatically enhanced properties, such as an abnormal increase in heat capacity at low concentration of NPs (e.g., C_p values 30% higher than the base material value). Understanding the thermo-physical behaviour of NFs is essential for their application as thermal energy storage systems. In this study, we analyse a sodium nitrate ionic system containing 1 wt%, 3 wt% and 7 wt% of SiO_2 NPs with different techniques like infrared thermography, infrared spectroscopy and differential scanning calorimetry (DSC) in order to shed light on the mechanism behind the increase of Cp. The themographies reveal the presence of a colder layer on top of the NF with 1 wt% of NPs whereas this layer does not appear at higher concentrations of NPs. The IR spectrum of this foamy top layer evidences the high amount of SiO_2 bonds suggesting the clustering of the NPs into this layer linked by the nitrate ions. The linking is enhanced by the presence of hydroxyls in the NPs' surface (i.e., hydroxylated NPs) that once mixed in the NF suffer ionic exchange between OH^- and NO_3^- species, leading to O_2–Si–O–NO_2 species at the interface where a thermal boundary resistance or Kapitza resistance appears (RT = 2.2 m^2 K kW^{-1}). Moreover, the presence of an exothermic reactive processes in the calorimetry of the mixture with 1 wt% of NPs evidences a reactive process (ionic exchange). These factors contribute to the heat capacity increase and thus, they explain the anomalous behaviour of the heat capacity in nanofluids.

Controlling pairing of π-conjugated electrons in 2D covalent organic radical frameworks via in-plane strain.

I. Alcón, R. Santiago, J. Ribas-Arino, M. Deumal, I. P. R. Moreira, S. T. Bromley.

Nat. Commun. *12* (2021) 1705.

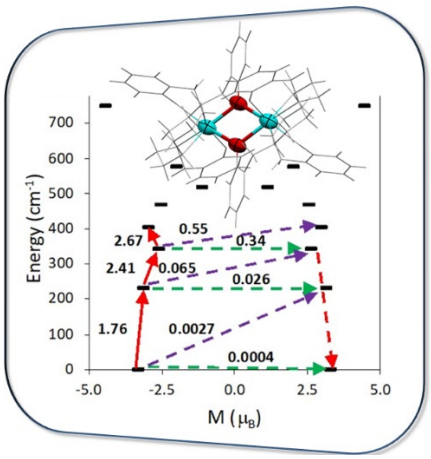


Controlling the electronic states of molecules is a fundamental challenge for future sub-nanoscale device technologies. π-conjugated bi-radicals are very attractive systems in this respect as they possess two energetically close, but optically and magnetically distinct, electronic states: the open-shell antiferromagnetic/paramagnetic and the closed-shell quinoidal diamagnetic states. While it has been shown that it is possible to statically induce one electronic ground state or the other by chemical design, the external dynamical control of these states in a rapid and reproducible manner still awaits experimental realization. Here, via quantum chemical calculations, we demonstrate that in-plane uniaxial strain of 2D covalently linked arrays of radical units leads to smooth and reversible conformational changes at the molecular scale that, in turn, induce robust transitions between the two kinds of electronic distributions. Our results pave a general route towards the external control, and thus technological exploitation, of molecular-scale electronic states in organic 2D materials.

Slow magnetic relaxation in dinuclear dysprosium and holmium phenoxide bridged complexes: A Dy_2 single molecule magnet with a high energy barrier.

M. Fondo, J. Corredoira-Vázquez, A. M. García-Deibe, J. Sanmartín-Matalobos, S. Gómez-Coca, E. Ruiz, E. Colacio.

Inorg. Chem. Front. *8* (2021) 2532-2541.

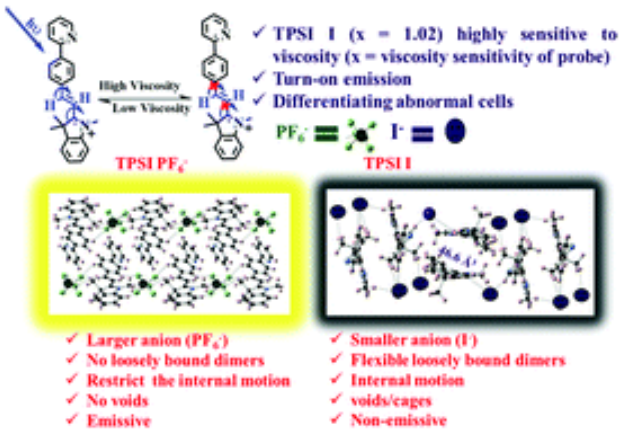


Dinuclear $[M(H_3L^{1,2,4})]_2$ (M = Dy, Dy_2; M = Ho, Ho_2) complexes were isolated from an heptadentate aminophenol ligand. The crystal structures of Dy_2·2THF, and the pyridine adducts Dy_2·2Py and Ho_2·2Py, show that the complexes are dinuclear, with unsupported double phenoxide bridges, and that the N_4O_4 environment of the Ln^{III} centres is distorted triangular dodecahedral. The magnetic analysis of Dy_2 and Ho_2 shows that Dy_2 is a single molecular magnet (SMM), with a thermal-activated zero-field effective energy barrier (U_{eff}) of 367.7 K, the largest barrier shown by double phenoxide-bridged dinuclear dysprosium complexes to date. Ho_2 is one of the scarce dinuclear complexes showing frequency-dependence for the out-of-phase component of susceptibility, although it does not even show field-induced SMM behaviour above 2 K. *Ab initio* calculations were performed in order to shed light on the magnetic dynamics of the complexes, and these studies support the experimental magnetic results.

Engineering a light-driven cyanine based molecular rotor to enhance the sensitivity towards a viscous medium.

V. Kachwal, A. Srivastava, S. Thakar, M. Zubiria-Ulacia, D. Gautam, S. K. P. Majumder, D. Casanova, R. Chowdhury, N. Rath, S. Mukherjee, P. Alemany, I, R.Laskar.

Mater. Adv. *2* (2021) 4804-4813.



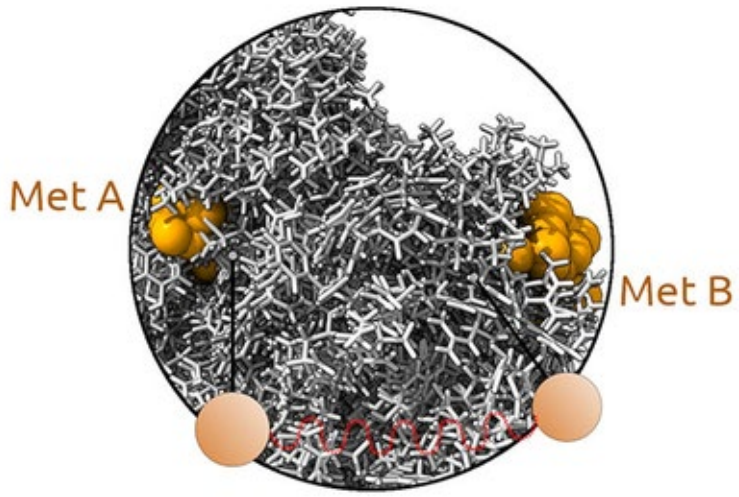
This article describes the enhanced sensitivity to a viscous medium by a molecular rotor based fluorophore (RBF), TPSI I. The TPSI I molecule is designed in such a way that it consists of a rotor and a fluorophore with a π-rich bridge between them. TPSI I is a light-responsive material in solution as well as in the solid state. The structural design of the molecule allows flexible rotation and photo-induced *cis–trans* isomerization both in the solid state as well as in solution. These combined attributes of TPSI I are responsible for the ultrasensitive viscosity response of the new material, which was verified through the Förster–Hoffmann equation. According to this equation, the derived '*x*' value is 1.02 (*x* is related to the sensitivity) which is the highest among the contemporary reports for RBFs. The facts were evidenced both by experimental as well as theoretical data. The ultrasensitivity towards viscosity was further analyzed in *in vitro* studies by detecting the subtle changes in the alteration of intracellular viscosity in normal and cancerous cells. An alteration of intracellular viscosity in cells treated with viscosity modulators was also confirmed using a previously well-established viscosity measurement technique, dynamic measurement through the piezoelectric patch. Our research offers a detailed mechanism to improve viscosity sensors and an efficient probe for detecting minute changes in intracellular viscosity.

LINE 3. BIOMEDICINE AND SOFT MATTER

A Methionine chemical shift based order parameter characterizing global protein dynamics.

S. Chashmniam, J. M. C. Teixeira, J. C. Paniagua, M. Pons.

ChemBioChem *22* (2021) 1001-1004.

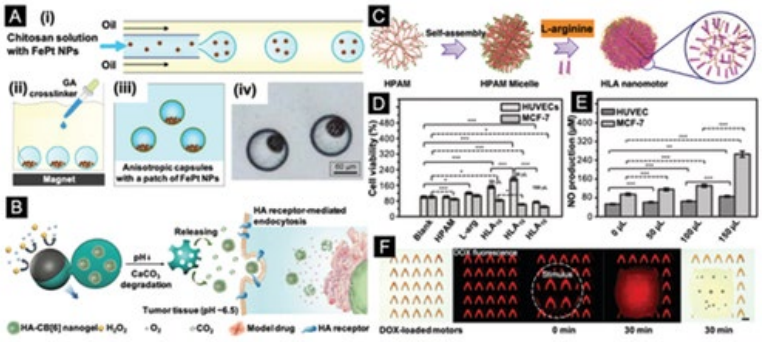


Coupling of side chain dynamics over long distances is an important component of allostery. Methionine side chains show the largest intrinsic flexibility among methyl-containing residues but the actual degree of conformational averaging depends on the proximity and mobility of neighbouring residues. The ^{13}C NMR chemical shifts of the methyl groups of methionine residues located at long distances in the same protein show a similar scaling with respect to the values predicted from the static X-ray structure by quantum methods. This results in a good linear correlation between calculated and observed chemical shifts. The slope is protein dependent and ranges from zero for the highly flexible calmodulin to 0.7 for the much more rigid calcineurin catalytic domain. The linear correlation is indicative of a similar level of side-chain conformational averaging over long distances, and the slope of the correlation line can be interpreted as an order parameter of the global side-chain flexibility.

Biodegradable small-scale swimmers for biomedical applications.

J. Llacer-Wintle, A. Rivas-Dapena, X. -Z. Chen, E. Pellicer, B. J. Nelson, J. Puigmartí-Luis, S. Pané.

Adv. Mater. *33* (2021) 2102049.

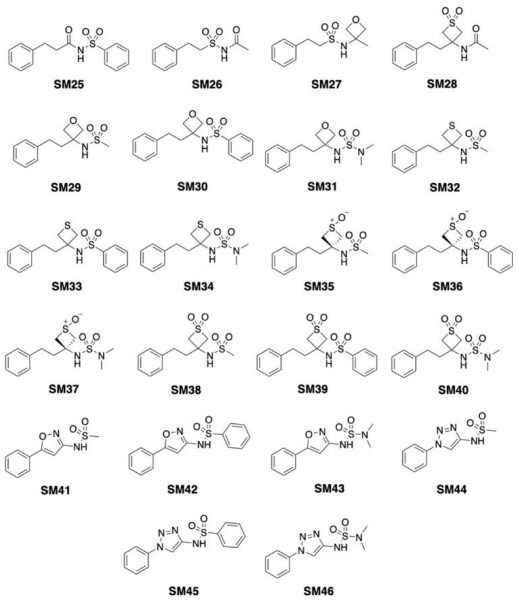


Most forms of biomatter are ephemeral, which means they transform or deteriorate after a certain time. From this perspective, implantable healthcare devices designed for temporary treatments should exhibit the ability to degrade and either blend in with healthy tissues, or be cleared from the body with minimal disruption after accomplishing their designated tasks. This topic is currently being investigated in the field of biomedical micro- and nanoswimmers. These tiny devices have the ability to move through fluids by converting physical or chemical energy into motion. Several architectures of these devices have been designed to mimic the motion strategies of nature's motile microorganisms and cells. Due to their motion abilities, these devices have been proposed as minimally invasive tools for precision healthcare applications. Hence, a natural progression in this field is to produce motile structures that can adopt, or even surpass, similar transient features as biological systems. The fate of small-scale swimmers after accomplishing their therapeutic mission is critical for the successful translation of small-scale swimmers' technologies into clinical applications. In this review, recent research efforts are summarized on the topic of biodegradable micro- and nanoswimmers for biomedical applications, with a focus on targeted therapeutic delivery.

Prediction of n-octanol/water partition coefficients and acidity constants (pK_a) in the SAMPL7 blind challenge with the IEFPCM-MST model.

A. Viayna A., S. Pinheiro, C. Curutchet, F. J. Luque, W. J. Zamora.

J. Comput.-Aided Mol. Des. *35* (2021) 803-811.

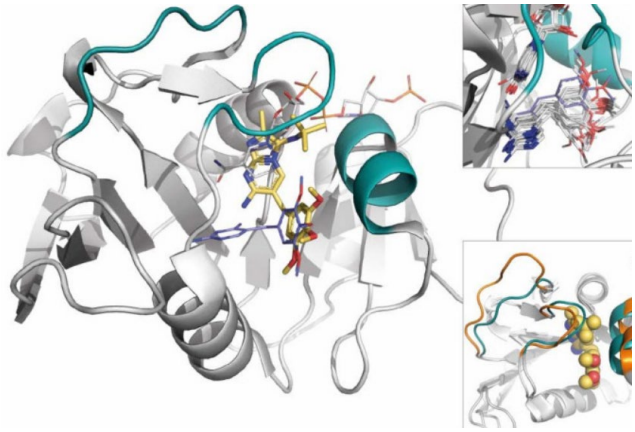


Within the scope of SAMPL7 challenge for predicting physical properties, the Integral Equation Formalism of the Miertus-Scrocco-Tomasi (IEFPCM/MST) continuum solvation model has been used for the blind prediction of n-octanol/water partition coefficients and acidity constants of a set of 22 and 20 sulfonamide-containing compounds, respectively. The log P and pK_a were computed using the B3LPYP/6-31G(d) parametrized version of the IEFPCM/MST model. The performance of our method for partition coefficients yielded a root-mean square error of 1.03 (log P units), placing this method among the most accurate theoretical approaches in the comparison with both globally (rank 8th) and physical (rank 2nd) methods. On the other hand, the deviation between predicted and experimental pK_a values was 1.32 log units, obtaining the second best-ranked submission. Though this highlights the reliability of the IEFPCM/MST model for predicting the partitioning and the acid dissociation constant of drug-like compounds compound, the results are discussed to identify potential weaknesses and improve the performance of the method.

New trimethoprim-like molecules: bacteriological evaluation and insights into their action.

M. Jorba, M. Pedrola, O. Ghashghaei, R. Herráez, L. Campos-Vicens, F. J. Luque, R. Lavilla, M. Viñas.

Antibiotics *10* (2021) 709.

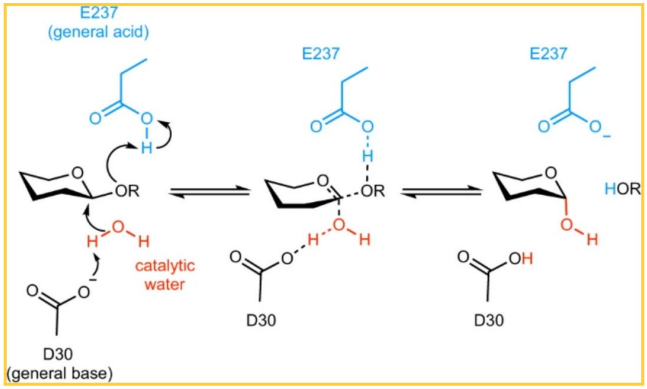


This work reports a detailed characterization of the antimicrobial profile of two trimethoprim-like molecules identified in previous studies. Both molecules displayed remarkable antimicrobial activity, particularly when combined with sulfamethoxazole. In disk diffusion assays on Petri dishes, both compounds showed synergistic effects with colistin. Specifically, in combinations with low concentrations of colistin, very large increases in the activities of compounds were determined, as demonstrated by alterations in the kinetics of bacterial growth despite only slight changes in the fractional inhibitory concentration index. The effect of colistin may be to increase the rate of antibiotic entry while reducing efflux pump activity. Both compounds were susceptible to extrusion by efflux pumps, whereas the inhibitor phenylalanine arginyl β-naphthylamide (PAβN) exerted effects similar to those of colistin. The interactions between the target enzyme (dihydrofolate reductase), the coenzyme nicotinamide adenine dinucleotide phosphate (NADPH), and the studied molecules were explored using enzymology tools and computational chemistry. A model based on docking results is reported.

Two distinct catalytic pathways for GH43 xylanolytic enzymes unveiled by X-ray and QM/MM simulations.

M. A. B. Morais, J. Coines, M. N. Domingues, R. A. S. Pirolla, C. C. C. Tonoli, C. R. Santos, J. B. L. Correa, F. C. Gozzo, C. Rovira, M. T. Murakami.

Nat. Commun. *12* (2021) 367.

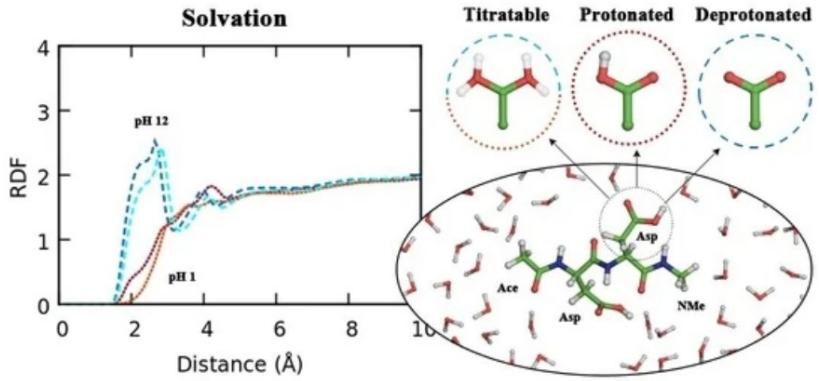


Xylanolytic enzymes from glycoside hydrolase family 43 (GH43) are involved in the breakdown of hemicellulose, the second most abundant carbohydrate in plants. Here, we kinetically and mechanistically describe the non-reducing-end xylose-releasing exo-oligoxylanase activity and report the crystal structure of a native GH43 Michaelis complex with its substrate prior to hydrolysis. Two distinct calcium-stabilized conformations of the active site xylosyl unit are found, suggesting two alternative catalytic routes. These results are confirmed by QM/MM simulations that unveil the complete hydrolysis mechanism and identify two possible reaction pathways, involving different transition state conformations for the cleavage of xylooligosaccharides. Such catalytic conformational promiscuity in glycosidases is related to the open architecture of the active site and thus might be extended to other exo-acting enzymes. These findings expand the current general model of catalytic mechanism of glycosidases, a main reaction in nature, and impact on our understanding about their interaction with substrates and inhibitors.

Unravelling constant pH molecular dynamics in oligopeptides with explicit solvation model.

C. Privat, S. Madurga, F. Mas, J. Rubio-Martinez.

Polymers *13* (2021) 3311.



An accurate description of the protonation state of amino acids is essential to correctly simulate the conformational space and the mechanisms of action of proteins or other biochemical systems. The pH and the electrochemical environments are decisive factors to define the effective pK_a of amino acids and, therefore, the protonation state. However, they are poorly considered in Molecular Dynamics (MD) simulations. To deal with this problem, constant pH Molecular Dynamics (cpHMD) methods have been developed in recent decades, demonstrating a great ability to consider the effective pK_a of amino acids within complex structures. Nonetheless, there are very few studies that assess the effect of these approaches in the conformational sampling. In a previous work of our research group, we detected strengths and weaknesses of the discrete cpHMD method implemented in AMBER when simulating capped tripeptides in implicit solvent. Now, we progressed this assessment by including explicit solvation in these peptides. To analyse more in depth the scope of the reported limitations, we also carried out simulations of oligopeptides with distinct positions of the titratable amino acids. Our study showed that the explicit solvation model does not improve the previously noted weaknesses and, furthermore, the separation of the titratable amino acids in oligopeptides can minimize them, thus providing guidelines to improve the conformational sampling in the cpHMD simulations.

III.2 PUBLICATION LIST

PUBLISHED ARTICLES

1. *Theory-guided enhancement of CO_2 reduction to ethanol on Ag-Cu tandem catalysts via particle-size effects.*
   Iyengar P., Kolb M.J., Pankhurst J., Calle-Vallejo F., Buonsanti R.
   ACS Catal. *11* (2021) 13330-13336.

2. *Thermodynamics and Kinetics of Molecular Hydrogen Adsorption and Dissociation on MXenes: Relevance to Heterogeneously Catalyzed Hydrogenation Reactions.*
   López M., Morales-García A., Viñes F., Illas F.
   ACS Catal. *11* (2021) 12850-12857.

3. *Carbon Capture and Usage by MXenes.*
   Morales-Salvador R., Gouveia J.D., Morales-García A., Viñes F., Gomes J.R.B., Illas F.
   ACS Catal. *11* (2021) 11248-11255.

4. *Asparagine Tautomerization in Glycosyltransferase Catalysis. The Molecular mechanism of protein O-Fucosyltransferase-1.*
   Piniello B., Lira-Navarrete E., Takeuchi H., Takeuchi M., Haltiwanger R.S., Hurtado-Guerrero R., Rovira C.
   ACS Catal. *11* (2021) 9926-9932.

5. *Supported Molybdenum Carbide Nanoparticles as an Excellent Catalyst for CO_2 Hydrogenation.*
   Figueras M., Gutiérrez R.A., Viñes F., Ramírez P.J., Rodriguez J.A., Illas F.
   ACS Catal. *11* (2021) 9679-9687.

6. *Toward efficient tandem electroreduction of CO_2 to methanol using anodized titanium.*
   Teh W.J., Piqué O., Low Q.H., Zhu W., Calle-Vallejo F., Yeo B.S.
   ACS Catal. *11* (2021) 8467-8475.

7. *Elucidating the Facet-Dependent Selectivity for CO_2 Electroreduction to Ethanol of Cu-Ag Tandem Catalysts.*
   Iyengar P., Kolb M.J., Pankhurst J.R., Calle-Vallejo F., Buonsanti R.
   ACS Catal. *11* (2021) 4456-4463.

8. *O-/ N-/ S-Specificity in Glycosyltransferase Catalysis: From Mechanistic Understanding to Engineering.*
   Teze D., Coines J., Fredslund F., Dubey K.D., Bidart G.N., Adams P.D., Dueber J.E., Svensson B., Rovira C., Welner D.H.
   ACS Catal. *11* (2021) 1810-1815.

9. *How Does Temperature Affect the Infrared Vibrational Spectra of Nanosized Silicate Dust?*
Guiu J.M., Escatllar A.M., Bromley S.T.
ACS Earth Space Chem. *5* (2021) 812-823.

10. *Amphiphilic Histidine-Based Oligopeptides Exhibit pH-Reversible Fibril Formation.*
Noble Jesus C., Evans R., Forth J., Estarellas C., Gervasio F.L., Battaglia G.
ACS Macro Lett. *10* (2021) 984-989.

11. *Piezoelectric Nanomaterials Activated by Ultrasound: The Pathway from Discovery to Future Clinical Adoption.*
Cafarelli A., Marino A., Vannozzi L., Puigmartí-Luis J., Pané S., Ciofani G., Ricotti L.
ACS Nano *15* (2021) 11066-11086.

12. *Pyrrole and Pyridine in the Water Environment—Effect of Discrete and Continuum Solvation Models.*
Zborowski K.K., Poater J.
ACS Omega *6* (2021) 24693-24699.

13. *2D Hexagonal Covalent Organic Radical Frameworks as Tunable Correlated Electron System.*
Santiago R., Alcón I., Ribas-Arino J., Deumal M., de P. R. Moreira I., Bromley S.T.
Adv. Funct. Mater. *31* (2021) 2004584.

14. *Biodegradable Small-Scale Swimmers for Biomedical Applications*.
Llacer-Wintle J., Rivas-Dapena A., Chen X.-Z., Pellicer E., Nelson B.J., Puigmartí-Luis J., Pané S.
Adv. Mater. *33* (2021) 2102049.

15. *Synthesis of 2D Porous Crystalline Materials in Simulated Microgravity.*
Contreras-Pereda N., Rodríguez-San-Miguel D., Franco C., Sevim S., Vale J.P., Solano E., Fong W.-K., Del Giudice A., Galantini L., Pfattner R., Pané S., Mayor T.S., Ruiz-Molina D., Puigmartí-Luis J.
Adv. Mater. *33* (2021) 2101777.

16. *A Submillimeter Continuous Variable Stiffness Catheter for Compliance Control.*
Lussi J., Mattmann M., Sevim S., Grigis F., De Marco C., Chautems C., Pané S., Puigmartí-Luis J., Boehler Q., Nelson B.J.
Adv. Sci. *8* (2021) 2101290.

17. *Helical Klinotactic Locomotion of Two-Link Nanoswimmers with Dual-Function Drug-Loaded Soft Polysaccharide Hinges.*
Wu J., Jang B., Harduf Y., Chapnik Z., Avci Ö.B., Chen X., Puigmartí-Luis J., Ergeneman O., Nelson B.J., Or Y., Pané S.
Adv. Sci. *8* (2021) 2004458.

18. *Room-Temperature Spin-Dependent Transport in Metalloporphyrin-Based Supramolecular Wires.*
Aragonès A.C., Martín-Rodríguez A., Aravena D., di Palma G., Qian W., Puigmartí-Luis J., Aliaga-Alcalde N., González-Campo A., Díez-Pérez I., Ruiz E.
Angew. Chem. Int. Ed. *60* (2021) 25958-25965.

19. *Exploiting Reaction-Diffusion Conditions to Trigger Pathway Complexity in the Growth of a MOF.*
Calvo Galve N., Abrishamkar A., Sorrenti A., Di Rienzo L., Satta M., D'Abramo M., Coronado E., de Mello A.J., Mínguez Espallargas G., Puigmartí-Luis J.
Angew. Chem. Int. Ed. *60* (2021) 15920-15927.

20. *Direct and Enantioselective Aldol Reactions Catalyzed by Chiral Nickel(II) Complexes.*
Kennington S.C.D., Teloxa S.F., Mellado-Hidalgo M., Galeote O., Puddu S., Bellido M., Romea P., Urpí F., Aullón G., Font-Bardia M.
Angew. Chem. Int. Ed. *60* (2021) 15307-15312.

21. *A Multifunctional Dysprosium-Carboxylato 2D Metall–Organic Framework.*
González J., Sevilla P., Gabarró-Riera G., Jover J., Echeverría J., Fuertes S., Arauzo A., Bartolomé E., Sañudo E.C.
Angew. Chem. Int. Ed. *60* (2021) 12001-12006.

22. *Selectivity Map for the Late Stages of CO and CO_2 Reduction to C_2 Species on Copper Electrodes.*
Piqué O., Low Q.H., Handoko A.D., Yeo B.S., Calle-Vallejo F.
Angew. Chem. Int. Ed. *60* (2021) 10784-10790.

23. *Bismuth Amides Mediate Facile and Highly Selective Pn–Pn Radical-Coupling Reactions (Pn=N, P, As).*
Oberdorf K., Hanft A., Ramler J., Krummenacher I., Bickelhaupt F.M., Poater J., Lichtenberg C.
Angew. Chem. Int. Ed. *60* (2021) 6441-6445.

24. *Cysteine Nucleophiles in Glycosidase Catalysis: Application of a Covalent β-L-Arabinofuranosidase Inhibitor.*
McGregor N.G.S., Coines J., Borlandelli V., Amaki S., Artola M., Nin-Hill A., Linzel D., Yamada C., Arakawa T., Ishiwata A., Ito Y., van der Marel G.A., Codée J.D.C., Fushinobu S., Overkleeft H.S., Rovira C., Davies G.J.
Angew. Chem. Int. Ed. *60* (2021) 5754-5758.

25. *Spin-Crossover Properties of an Iron(II) Coordination Nanohoop.*
Heras Ojea M.J., Van Raden J.M., Louie S., Collins R., Pividori D., Cirera J., Meyer K., Jasti R., Layfield R.A.
Angew. Chem. Int. Ed. *60* (2021) 3515-3518.

26. *How Oxygen Binding Enhances Long-Range Electron Transfer: Lessons From Reduction of Lytic Polysaccharide Monooxygenases by Cellobiose Dehydrogenase.*
Wang Z., Feng S., Rovira C., Wang B.
Angew. Chem. Int. Ed. *60* (2021) 2385-2392.

27. *New trimethoprim-like molecules: Bacteriological evaluation and insights into their action.*
Jorba M., Pedrola M., Ghashghaei O., Herráez R., Campos-Vicens L., Luque F.J., Lavilla R., Viñas M.
Antibiotics *10* (2021) 709.

28. *CO oxidation activity of Pt/CeO_2 catalysts below 0 °C: platinum loading effects.*
Boronin A.I., Slavinskaya E.M., Figueroba A., Stadnichenko A.I., Kardash T.Y., Stonkus O.A., Fedorova E.A., Muravev V.V., Svetlichnyi V.A., Bruix A., Neyman K.M.
Appl. Catal. B: Environ. *286* (2021) 119931.

29. *How symmetry factors cause potential- and facet-dependent pathway shifts during CO_2 reduction to CH_4 on Cu electrodes.*
Rendón-Calle A., Low Q.H., Hong S.H.L., Builes S., Yeo B.S., Calle-Vallejo F.
Appl. Catal. B: Environ. *285* (2021) 119776.

30. *Chelation enforcing a dual gold configuration in the catalytic hydroxyphenoxylation of alkynes.*
Escayola S., Poater J., Ramos M., Luque-Urrutia J.A., Duran J., Simon S., Solà M., Cavallo L., Nolan S.P., Poater A.
Appl. Organomet. Chem. *35* (2021) e6362.

31. *Magnetoelectric coupling in micropatterned $BaTiO_3/CoFe_2O_4$ epitaxial thin film structures: Augmentation and site-dependency.*
Kim D., Rossell M.D., Campanini M., Erni R., Puigmartí-Luis J., Chen X.-Z., Pané S.
Appl. Phys. Lett. *119* (2021) 12901.

32. *The Ti_2CO_2 MXene as a nucleobase 2D sensor: A first-principles study.*
Gouveia J.D., Novell-Leruth G., Viñes F., Illas F., Gomes J.R.B.
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128. *Self-Assembly Hydrosoluble Coronenes: A Rich Source of Supramolecular Turn-On Fluorogenic Sensing Materials in Aqueous Media.*
Romero D.C., Calvo-Gredilla P., García-Calvo J., Diez-Varga A., Cuevas J.V., Revilla-Cuesta A., Busto N., Abajo I., Aullón G., Torroba T.
Org. Lett. *23* (2021) 8727-8732.

129. *Inhibition Ability of Natural Compounds on Receptor-Binding Domain of SARS-CoV2: An In Silico Approach.*
Nedyalkova M., Vasighi M., Sappati S., Kumar A., Madurga S., Simeonov V.
Pharmaceuticals *14* (2021) 1328.

130. *Evaluation of the interactions between human serum albumin (Hsa) and non-steroidal anti-inflammatory (nsaids) drugs by multiwavelength molecular fluorescence, structural and computational analysis.*
Amézqueta S., Beltrán J.L., Bolioli A.M., Campos-vicens L., Luque F.J., Ràfols C.
Pharmaceuticals *14* (2021) 214.

131. *Vibrational energy relaxation of a diatomic molecule in a superfluid helium nanodroplet: Influence of the nanodroplet size, interaction energy and energy gap.*
Blancafort-Jorquera M., González M.
Phys. Chem. Chem. Phys. *23* (2021) 25961-25973.

132. *Low-dimensional HfS_2 as SO_2 adsorbent and gas sensor: Effect of water and sulfur vacancies.*
Bouheddadj A., Ouahrani T., Kanhounnon W.G., Reda B.M., Bedrane S., Badawi M., Morales-García Á.
Phys. Chem. Chem. Phys. *23* (2021) 23655-23666.

133. *Monitoring the active sites for the hydrogen evolution reaction at model carbon surfaces.*
Kluge R.M., Haid R.W., Stephens I.E.L., Calle-Vallejo F., Bandarenka A.S.
Phys. Chem. Chem. Phys. *23* (2021) 10051-10058.

134. *Twistable dipolar aryl rings as electric field actuated conformational molecular switches.*
Jutglar Lozano K., Santiago R., Ribas-Arino J., Bromley S.T.
Phys. Chem. Chem. Phys. *23* (2021) 3844-3855.

135. *Fragment dissolved molecular dynamics: A systematic and efficient method to locate binding sites.*
Privat C., Granadino-Roldán J.M., Bonet J., Santos Tomas M., Perez J.J., Rubio-Martinez J.
Phys. Chem. Chem. Phys. *23* (2021) 3123-3134.

136. *Magnetic anisotropy in YbIII complex candidates for molecular qubits: a theoretical analysis.*
Amoza M., Gómez-Coca S., Ruiz E.
Phys. Chem. Chem. Phys. *23* (2021) 1976-1983.

137. *Assigning XPS features in B,N-doped graphene: Input from: Ab initio quantum chemical calculations.*
Costa R., Morales-García Á., Figueras M., Illas F.
Phys. Chem. Chem. Phys. *23* (2021) 1558-1565.

138. *Healthcare workers hospitalized due to COVID-19 have no higher risk of death than general population. Data from the Spanish SEMI-COVID-19 Registry.*
Díez-Manglano J., Solís-Marquínez M.N., García A.Á., Alcalá-Rivera N., Riesco I.M., Aseguinolaza M.G., Pérez J.L.B., Bailón M.M., Ruiz A.-E.L.-I., Gómez M.G., Cilleros C.M., Fontan P.M.P., Vázquez L.A., Encinar J.C.B., Boixeda R., and col.
PLoS ONE *16* (2021) e0247422.

139. *Nickel(II) salicylaldiminates: Re-visiting a classic.*
Saechio S., Clérac R., Murray K.S., Phonsri W., Ruiz E., Harding P., Harding D.J.
Polyhedron *205* (2021) 115321.

140. *Non-monotonic behavior of weak-polyelectrolytes adsorption on a cationic surface: A Monte Carlo simulation study.*
Narambuena C.F., Blanco P.M., Rodriguez A., Rodriguez D.E., Madurga S., Garcés J.L., Mas F.
Polymers *13* (2021) 123170.

141. *Unveiling the effect of low ph on the sars-cov-2 main protease by molecular dynamics simulations.*
Barazorda-Ccahuana H.L., Nedyalkova M., Mas F., Madurga S.
Polymers *13* (2021) 3823.

142. *Unravelling constant ph molecular dynamics in oligopeptides with explicit solvation model.*
Privat C., Madurga S., Mas F., Rubio-Martinez J.
Polymers *13* (2021) 3311.

143. *On the use of the discrete constant pH molecular dynamics to describe the conformational space of peptides.*
Privat C., Madurga S., Mas F., Rubio-Martínez J.
Polymers *13* (2021) 99.

144. *Concurrent mutations in RNA-dependent RNA polymerase and spike protein emerged as the epidemiologically most successful SARS-CoV-2 variant.*
Ilmjärv S., Abdul F., Acosta-Gutiérrez S., Estarellas C., Galdadas I., Casimir M., Alessandrini M., Gervasio F.L., Krause K.-H.
Sci. Rep. *11* (2021) 13705.

145. *Understanding the abnormal thermal behavior of nanofluids through infrared thermography and thermo-physical characterization.*
Svobodova-Sedlackova A., Calderón A., Barreneche C., Gamallo P., Fernández A.I.
Sci. Rep. *11* (2021) 4879.

146. *Influence of macromolecular crowding on the charge regulation of intrinsically disordered proteins.*
Blanco P.M., Madurga S., Garcés J.L., Mas F., Dias R.S.
Soft Matter. *17* (2021) 655-669.

147. *Prediction of partition coefficients in SDS micelles by DFT calculations.*
Saranjam L., Fuguet E., Nedyalkova M., Simeonov V., Mas F., Madurga S.
Symmetry *13* (2021) 1750.

148. *Effect of Cr^{3+} doped on electronic and magnetic properties of $SrFe_{12}O_{19}$ by first-principles study.*
Hmok H.L., Betancourt I., Martínez-Aguilar E., Ribas-Ariño J., Herrera O.R.
Theor. Chem. Acc. *140* (2021) 136.

149. *The energy components of the extended transition state energy decomposition analysis are path functions: the case of water tetramer.*
Solà M., Duran M., Poater J.
Theor. Chem. Acc. *140* (2021) 33.

150. *Concepts, models, and methods in computational heterogeneous catalysis illustrated through CO_2 conversion.*
Morales-García Á., Viñes F., Gomes J.R.B., Illas F.
WIREs Comput. Mol. Sci. *11* (2021) e1530.

BOOK CHAPTERS AND PROCEEDINGS

1. *Synchronous flipped classroom in stem subjects [Clase invertida síncrona en asignaturas stem].*
   Maya Díaz C., Iglesias Sigüenza J., Giménez X.
   Revista de Educacion (2021) 15-39.

III.3 OTHER ACTIVITIES

PHD THESES 2021

1. *Nanostructured transition metal carbides as potential catalysts for greenhouse gases conversion.*
   Marc Figueras Valls
   PhD program: Theoretical Chemistry and Computational Modelling.
   Faculty of Chemistry, University of Barcelona.
   Supervisor/s: F. Viñes, F. Illas.
   December 2021.

2. *Computational modeling of transition metals carbides with relevant to nanotechnology and catalysis.*
   Juan José Piñero Vargas
   PhD program: Theoretical Chemistry and Computational Modelling.
   Faculty of Chemistry, University of Barcelona.
   Supervisor/s: F. Viñes, S. Bromley.
   December 2021.

3. *Advanced modelling of metallic nanomaterials for catalysis.*
   Lorena Vega Domínguez
   PhD program: Theoretical Chemistry and Computational Modelling.
   Faculty of Chemistry, University of Barcelona.
   Supervisor/s: K. Neyman, F. Viñes.
   December 2021.

4. *Exploring molecular mechanisms of key targets in metabolic and infectious diseases.*
   Elnaz Aledavood
   PhD program: Biotechnology.
   Faculty of Pharmacy and Food Sciences, University of Barcelona.
   Supervior/s: C. Estarellas, F. J. Luque.
   October 2021.

5. *Cosymlib: a Python library for continuous symmetry measures and its application to problems in structural chemistry.*
   Efrem Bernuz Fito
   PhD program: Theoretical Chemistry and Computational Modelling.
   Faculty of Chemistry, University of Barcelona.
   Supervisor/s: P. Alemany.
   July 2021.

6. *Controlled self-assembly employing microfluidic tools: pathway selection in materials synthesis and processing.*
Semih Sevim
PhD program: DDC Science, Chemistry, Technology, Medicine and Applied Sciences, Chem. Engineering.
ETH Zurich.
Supervisor/s: A. DeMello, J. Puigmartí, S. Pané.
April 2021.

MASTER THESES 2021

1. *Optimization of the separation of methanol and methyl acetate using pressure swing distillation.*
Iván Río Romo
MSc program: Chemical Engineering.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: Alexandra Plesu Popescu, Víctor Manso Álvarez.
July 2021.

2. *Contribution to the construction and validation of a prototype of a CO_2 adsorption filter of a vehicle exhaust gases using zeolites.*
Karim Tarik Gascón
MSc program: Chemical Engineering.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: Alexandra Plesu Popescu, Jordi Bonet-Ruiz.
July 2021.

3. *Contribution to the study of extractive rectification.*
Carlos Ramírez González
MSc program: Chemical Engineering.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: Alexandra Plesu Popescu, Jordi Bonet-Ruiz.
July 2021.

4. *Recovery of aqueous solvents from the pharmaceutical industry: isopropanol and ethyl acetate.*
Oriol Yáñez Gaya
MSc program: Chemical Engineering.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: Alexandra Plesu Popescu, Jordi Bonet-Ruiz.
July 2021.

5. *Basic concepts of control of a reactive rectification column with lateral decanter.*
Roger Fabregat Feliu
MSc program: Chemical Engineering.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: Jordi Bonet-Ruiz, David Curcó.
July 2021.

6. *Critical comparision of alternative processes for chemical absorption of CO_2.*
Ana Elguea
MSc program: Environmental Engineering.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: Alexandra Plesu Popescu, Jordi Bonet-Ruiz.
July 2021

7. *Determining the structure and oxidation state of ceria-supported PtyOx particles un-der reactive environments.*
Jon Eunan Quinlivan Domínguez
MSc program: Theoretical Chemistry and Computational Modeling
Faculty of Chemistry, University of Barcelona.
Supervisor/s: Albert Bruix
July 2021.

8. *Rotational relaxation in superfluid helium nanodroplets. The case of HCl and isotopic variants.*
Eloi Sánchez Ambrós
MSc program: Atomistic and Multiscale Computational Modelling in Physics, Chemistry and Biochemistry. Interuniversitary Master (UB-UPC).
Faculty of Chemistry, University of Barcelona.
Supervisor/s: Miguel González Pérez.
July 2021.

9. *Computational Fluid Dynamics Study of exhaust gases cooling.*
Alba Gil Malibern
MSc program: Chemical Engineering.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: Alexandra Plesu Popescu, Rubén Cabello Gallego.
February 2021.

10. *Efficiency study of reaction-separation recycle systems.*
Kevin Marín González
MSc program: Chemical Engineering.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: Alexandra Plesu Popescu, Jordi Bonet-Ruiz.
February 2021.

11. *Study of the drug-resistant S31N mutant of the influenza A virus M2 channel thorugh constant-pH Molecular Dynamics simulations*
Beatrice Selmi
Tesi di Laurea
University of Bologna (Italy)
Supervisor/s: M. Massetti, R. Ocello, F. J. Luque
February 2021

SCIENTIFIC CONFERENCES AND MEETINGS 2021

Recent Advances in Modelling Rare Events (RARE2021)
online, 15-17th December 2021

QM/MM metadynamics simulations of novel chemical reactions in glycoprocessing enzymes (invited talk)
C. Rovira

International Conference on Frontiers in Electrocatalytic Transformations (INTERECT)
Valencia (Spain), November 2021

Toward predictive and affordable computational models for CO_2 electroreduction (keynote talk)
F. Calle-Vallejo

EXTREME Winterschool "Innovations and applied aspects of colloid and interface science"
online, 22-23rd November 2021

Introduction to machine learning for chemists (invited talk)
A. Bruix

13th European Conference on Computational and Theoretical Chemistry
online, 18-19th November 2021

M. Deumal *(organizing committee)*

I Simposio de Jóvenes Investigadores de la Real Academia Nacional de Medicina
Madrid (Spain), 17th November 2021

Mecanismo de reconocimiento molecular de la trimetil-lisina a partir de sistemas aromáticos fluorados (invited talk)
J. Poater

International Conference on Carbon Chemistry and Materials
Rome (Italy), 15th November 2021

Non-covalent nido-cage π-ring interaction (invited talk)
J. Poater

Catalysis, Chemical Engineering & Technology
online, 15th November 2021

Teaching iron to perform like palladium in cross coupling reactions (invited talk)
J. Poater

BeMAGIC Winter School: Magnetoelectricity in biomedicine: healthcare for the 21st century
online, 8-12th November 2021

Microfluidic technologies for chemistry and materials engineering (invited talk)
J. Puigmartí-Luis

Computational methods in photosynthesis
online, Amsterdam (Netherlands), 8-11th November 2021

Determination of the energy ladder in cryptophyte antenna complexes from multiscale simulations (invited talk)
C. Curutchet

Spanish Network of Biocatalysis (RTBIOCAT)
online, 28th October 2021

Biocatalysis cicle (invited talk)
C. Rovira

KEN2021 - XLIV
online, 26th October 2021

Exploiting controlled reaction-diffusion conditions for materials synthesis: Looking back…with a view to the future… (invited talk)
J. Puigmartí-Luis

Midi MINATEC
online, 15th October 2021

Microfluidic technologies for materials engineering: Looking back…with a view to the future… (invited talk)
J. Puigmartí-Luis

12th International Congress "Biomaterials and Nano-biomaterials: Recent Advances Safety - Toxicology and Ecology Issues"
online, 1st October 2021

Microfluidic technologies for chemistry, materials science and biotechnology (invited talk)
J. Puigmartí-Luis

Symposium of the Spanish Royal Society of Chemistry
online, 27-30th September 2021

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

Solar Power and Chemical Energy Systems (SolarPACES)
online, 27th September -1st October 2021

Specific heat capacity of nanofluids: a sampling study (oral communication)
A. Svobodova-Sedlakova, C. Barreneche, P. Gamallo, A. I. Fernández

EUROPIN Summer School on Drug Design
online, Wien (Austria), 13-17th September 2021

From simple models of solvation to applications in target druggability and screening of drug-like compounds (invited talk)
F. Javier Luque

RES Virtual Users Conference 2021 "Innovations and applied aspects of colloid and interface science"
online, 16-17th September 2021

Predicting the structure and oxidation state of complex materials under reaction conditions (invited talk)
A. Bruix

15th RES Users Conference
online, 16th September 2021

Revealing the key factors of direct activation mechanism of AMPK based on isoformdependent complex (invited lecture)
C. Estarellas

3rd European Symposium on Nanofluids (ESNf)
online, Iasi (Romania), 9-10th September 2021

Thermo-physical properties of nanofluids: A sampling study (oral communication)
A. Svobodova-Sedlakova, C. Barreneche, P. Gamallo, A. I. Fernández

Life Sciences Department and Bio4InfoWomen seminar series
online, Barcelona (Spain) 2nd September 2021

Using computers to understand how carbohydrates are processed in Nature (invited talk)
C. Rovira

72nd Annual Meeting of the ISE
Jeju Island (South Korea), August-September 2021

Toward accurate and affordable computational models for the electroreduction of CO_2 (keynote talk)
F. Calle-Vallejo

Smart Composites International School and IV International Baltic Conference on Magnetism (IBCM-2021)
Svetlogorsk (Russia), 29th August – 2nd September 2021

In-silico design of bimetallic nanocrystallites to speed-up their manufacturing (invited talk)
K. Neyman

St. Jude Children's Research Hospital. Chemical Biology and Therapeutics Department. Memphis
online, Memphis (USA) 5th August 2021

Using computers to understand how carbohydrates are processed in Nature (invited talk)
C. Rovira

Beijing Institut of Technology (BIT)
online, 3rd August 2021

Is chemistry the only key strategy to successfully control materials synthesis as desired? (invited talk)
J. Puigmartí-Luis

EXTREME Workshop "Innovations and applied aspects of colloid and interface science"
St. Constantine and Helena (Bulgaria), 18-21st July 2021

Addressing the complexity of nanostructured materials in catalysis modelling (invited talk)
A. Bruix

International Workshop "Colloid and interface research & innovations"
Varna (Bulgaria), 18-21st July 2021

Metal/metal-oxide interface effects in nanomaterials for catalysis and energy technologies: DFT modelling versus experiment (plenary lecture)
K. Neyman

EXTREME Summerschool "Innovations and applied aspects of colloid and interface science"
St. Constantine and Helena (Bulgaria), 14-16th July 2021

Modelling of solid catalysts based on first principles: from active site characterization to reaction simulations (invited talk)
A. Bruix

CECAM Workshop "Multi-approach modeling of alloy nanoparticles: from non-equilibrium synthesis to structural and functional properties"
online, Lyon (France), 7-8th July 2021

Bimetallic nanoalloys of Pt and Pd with Au, Ag and Cu: Chemical orderings and properties from DFT calculations combined with a topological approach (invited lecture)
K. Neyman

7th International Iberian Biophysics Congress
online, 14-16th June 2021

Decoding Mechanisms of Allosteric Regulation: AMPK as an Energy Sensor in the Cell (invited talk)
F. Javier Luque

CECAM Flagship Workshop Nonequilibrium dynamical solvent effects on excited states: from spectroscopy to photoreactivity
online, Paris (France), 14-17th June 2021

Understanding solvent effects on electronic energy transfer from multiscale quantum/classical models (invited talk)
C. Curutchet

15th International Virtual Conference on Energy Storage (ENERSTOCK)
online, Ljubljana (Slovenia), 9-11th June 2021

Nanofluids study through infrared thermography and physico-chemical characterization (oral communication)
A. Svobodova-Sedlakova, A. Calderón, C. Barreneche, P. Gamallo, A. I. Fernández

29th edition of the International Symposium on Molecular Beams (ISMB2021)
online, 1-2nd July 2021

Quasiclassical trajectory study of the dynamics of the $O + D_2^+ \longrightarrow OD^+ + D$ gas phase reaction (oral communication)
P. Gamallo, M. Paniagua, M. González

7th European Chemical Biology Symposium (7ECBS)
online, 26-28th May 2021

Using computers to understand how carbohydrates are processed in nature (invited talk)
C. Rovira

14th European School on Molecular Nanoscience
Alicante (Spain), 24-27th May 2021

Simulated microgravity conditions for materials synthesis (invited talk)
J. Puigmartí-Luis

6th International School-Conference on Catalysis for Young Scientists "Catalyst Design: from molecular to industrial level"
Novosibirsk (Russia), 16-19th May 2021

K. M. Neyman *(organizing committee)*

CECAM Flagship School on Kinetics and Dynamics of Chemical Reactions
online, Zaragoza (Spain), 26-30th April 2021

P. Gamallo *(organizing committee)*

Universidad Europea de Madrid
online, 16th April 2021

Molecular Dynamics: A tool to understand the biochemical processes of the cell (invited talk)
F. Javier Luque

29th Topical Meeting of the ISE
online, April 2021

Outlining the optimization of electrocatalysts for water splitting (invited talk)
F. Calle-Vallejo

RSC Desktop Seminar Lectureship with PCCP
online, March 2021

Designing water splitting catalysts using rules of thumb: advantages, dangers and alternatives (invited talk)
F. Calle-Vallejo

BioExcel Virtual Workshop on Best Practices in QM/MM Simulation of Biomolecular Systems
online, 12th January 2021

Modeling catalytic mechanisms in carbohydrate-active enzymes with QM/MM MD methods (invited talk)
C. Rovira

RESEARCH STAYS IN RECOGNIZED CENTERS

Lozano, P.	**University of Technology, Gothemburg (Sweden)** Sept-Dec 2021
López, M.	**University of Druisburg-Essen, Essen (Germany)** Aug-Sept 2021
Puigmartí, J.	**Laboratoire des Matériaux et du Génie Physique (LMGP), Grenoble, (France)** Oct-Dec 2021

PARTICIPATION IN COMPETITIVE FUNDED RESEARCH PROJECTS

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

ALLODD – Allostery in Drug Discovery.
X. Barril, C. Curutchet, University of Barcelona
H2020-MSCA-ITN-2020, 2021-2025
European Union
Amount: 227.024 EUR

Tiny devices delivering drugs precisely where needed (ANGIE FET Proactive).
J. L. Puigmartí, University of Barcelona
H2020-EIC- FETPROACT 2021-2024
European Union
Amount: 555.000 EUR

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

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

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

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

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

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

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

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

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

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

Ammonia recovery from animal slurries by means of a novel selective membrane.
J. Mata Álvarez, F. Mas, University of Barcelona
Private company contract, 2021-2022
INDUKERN-REVAGO
Amount: 88.354 EUR

Identification of allosteric effectors causin depletion of pathology-related proteins.
J. Juárez-Jiménez, X. Barril, University of Barcelona
Private company contract, 2021-2022
INDUKERN-REVAGO
Amount: 53.600 EUR

Modelización Computacional de Materials Interruptor.
J. Cirera, University of Barcelona
PID2020-115165GB-I00, 2021-2024
Spanish Ministry of Science, Innovation and Universities
Amount: 66.913 EUR

Modelización de la inter-relación entre estructura y espectroscopía en biosistemas.
C. Curutchet, University of Barcelona
PID2020-115812GB-I00, 2021-2024
Spanish Ministry of Science, Innovation and Universities
Amount: 96.800 EUR

Explorando nuevas estratègies en enfermedades víricas y tuberculosis: plasticidad conformacional, resistència a mutacions y modificación química pseudoirreversible.
F. J. Luque, University of Barcelona
PID2020-117646RB-I00, 2021-2024
Spanish Ministry of Science, Innovation and Universities
Amount: 170.610 EUR

Síntesis y crecimiento controlado de estructures metal-orgánicas poroses con tecnologies microfluídicas.
J. L. Puigmartí, University of Barcelona
PID2020-116612RB-C33, 2021-2024
Spanish Ministry of Science, Innovation and Universities
Amount: 151.250 EUR

Materiales basados en moléculas de capa abierta: comprensión y predicción de sus estructures y propiedades físicas a través de la modelización computacional.
J. Ribas, University of Barcelona
PID2020-117803GB-I00, 2021-2024
Spanish Ministry of Science, Innovation and Universities
Amount: 121.000 EUR

Simulación computacional de mecanismos catalíticos en enzimas actives en carbohidratos mediante técnicas de dinàmica molecular QM/MM.
C. Rovira, University of Barcelona
PID2020-118893GB-I00, 2021-2024
Spanish Ministry of Science, Innovation and Universities
Amount: 145.200 EUR

Bases moleculares de cooperatividad química en complejos ternarios de interés terapéutico.
J. Juárez-Jiménez, University of Barcelona
PID2020-115683GA-I00, 2021-2024
Spanish Ministry of Science, Innovation and Universities
Amount: 84.700 EUR

Doctorats industrials 2020. Empresa: Pharmacelera S.L.
F. J. Luque, University of Barcelona
2020DI92, 2021-2024
Agency for Management of University and Research Grants
Amount: 33.960 EUR

PATENT OR MARK APPLICATION

Nanoreactors for the synthesis of porous crystalline materials.
J. Puigmarti-Luis, F. Juan Zamora Abandes, C. Franco Pujante, D. Rodriguez San Miguel, A. Sorrenti
US Patent App.
17/255,121, 2021

Institut de Química Teòrica i Computacional