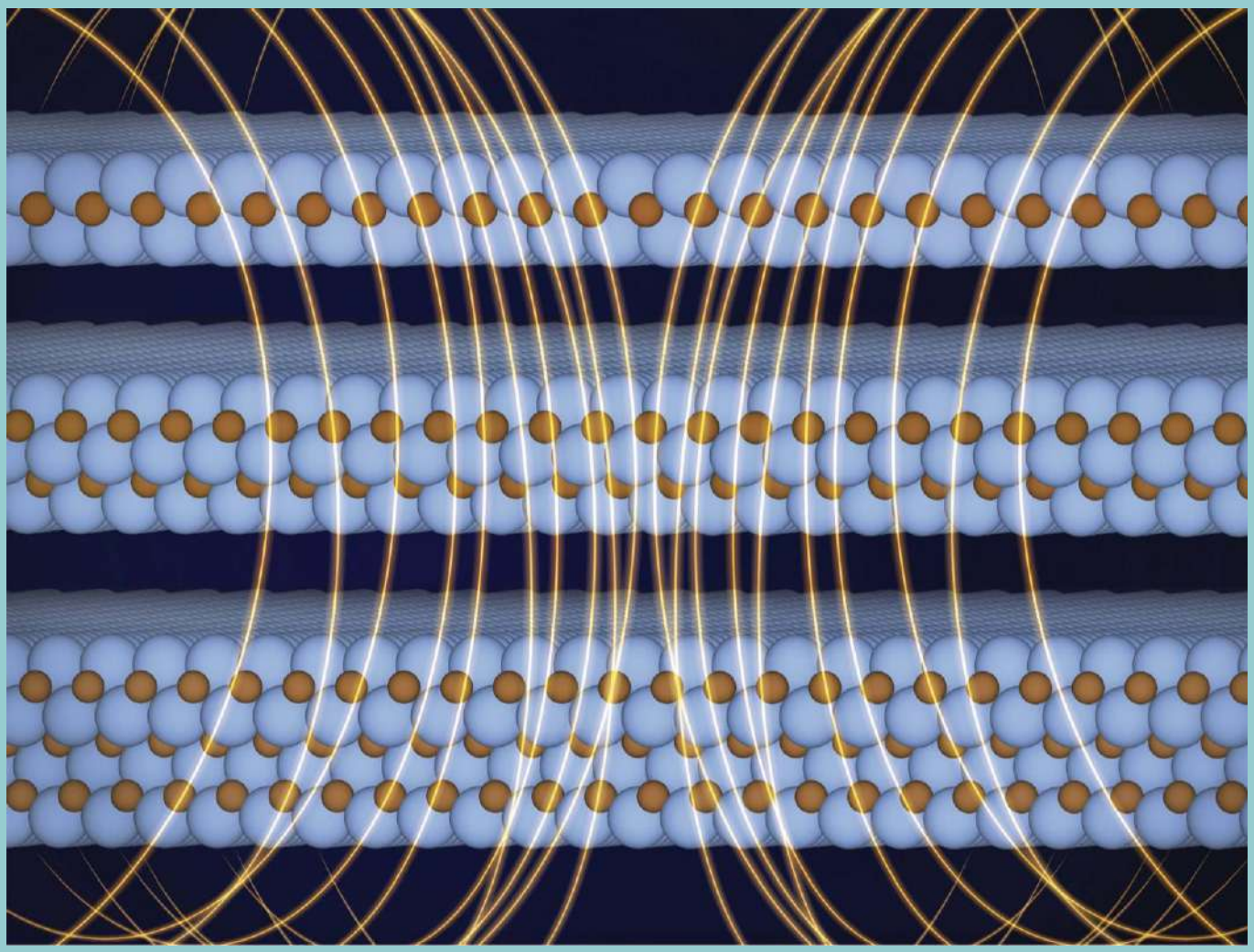
iqtc

Institut de Química Teòrica
i Computacional

EXCELENCIA
MARÍA
DE MAEZTU

UNIVERSITAT DE
BARCELONA

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

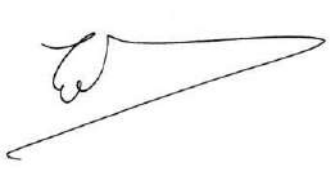


Activity Report 2023

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. The year 2022 has meant an important consolidation of our Institute with the renewal of the María de Maeztu seal of excellence for four more years. 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 main 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. A primary objective now is to enhance collaboration among the Institute's groups, especially the new incorporations that will contribute to strengthening the structure of the center.

Computational chemistry is in a period of profound change. The inclusion of methods based on Artificial Intelligence will mean a drastic change in the way of understanding Science, and in how to approach scientific challenges. In our Institute, many groups are currently using this type of tools, and this will provide new challenges and the ability to address more complex systems. 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

REPORT CONTENT

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.

Direction Team

The IQTCUB direction team during 2023 has been:

Prof. Eliseo Ruiz Sabin	*Director*
Prof. Francesc Viñes Solana	*Secretary*
Prof. Francesc Illas Riera	*Board member*

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. **Catalysis, energy and environment**

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 for emergent technologies**

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. Biocatalysis and drug discovery

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.

IQTCUB MEMBERS

IQTCUB involves a more than 140 professors and researchers: The full list of members of IQTCUB (including the corresponding academic situation and affiliation within UB) is provided below.

Full Professors

Surname	Name	Country	Gender	Depart. Unit
Alemany I Canher	Pere	Spain	Male	Department of Materials Science and Physical Chemistry
Aullón López	Gabriel	Spain	Male	Department of Inorganic and Organic Chemistry
Barril	Xavier	Spain	Male	Department of Pharmacy and Pharmaceutical Technology, and Physical Chemistry
Bofill Villà	Josep Maria	Spain	Male	Department of Inorganic and Organic Chemistry
Curutchet Barat	Carles	Spain	Male	Department of Pharmacy and Pharmaceutical Technology, and Physical Chemistry
Deumal Solé	Mercè	Spain	Female	Department of Materials Science and Physical Chemistry
González Pérez	Miguel	Spain	Male	Department of Materials Science and Physical Chemistry
Illas Riera	Francesc	Spain	Male	Department of Materials Science and Physical Chemistry
Luque Garriga	Francisco Javier	Spain	Male	Department of Nutrition, Food Sciences and Gastronomy Basic Sciences Applied to Food Science
Mas Pujadas	Francesc	Spain	Male	Department of Materials Science and Physical Chemistry
Reigada Sanz	Ramon	Spain	Male	Department of Materials Science and Physical Chemistry

Rubio Martínez	Jaime	Spain	Male	Department of Materials Science and Physical Chemistry
Ruiz Sabin	Eliseo	Spain	Male	Department of Inorganic and Organic Chemistry
Sayós Ortega	Ramon	Spain	Male	Department of Materials Science and Physical Chemistry
Sousa Romero	María del Carmen	Spain	Female	Department of Materials Science and Physical Chemistry

Aggregate Professors

Surname	Name	Country	Gender	Depart. Unit
Bidon-Chanal Badia	Axel	Spain	Male	Department of Nutrition, Food Sciences and Gastronomy Basic Sciences Applied to Food Science
Bonet Ruiz	Jordi	Spain	Male	Department of Chemical Engineering and Analytical Chemistry
Gamallo Belmonte	Pablo	Spain	Male	Department of Materials Science and Physical Chemistry
Limburg	Bart	Holland	Male	Department of Inorganic and Organic Chemistry
Madurga Díez	Sergio	Spain	Male	Department of Materials Science and Physical Chemistry
Plesu Popescu	Alexandra	Spain	Female	Department of Chemical Engineering and Analytical Chemistry
Ribas Ariño	Jordi	Spain	Male	Department of Materials Science and Physical Chemistry
Viñes Solana	Francesc	Spain	Male	Department of Materials Science and Physical Chemistry

Associate Professors

Surname	Name	Country	Gender	Depart. Unit
Cremades Marti	Eduard	Spain	Male	Department of Inorganic and Organic Chemistry
De Pinho Ribeiro Moreira	Ibério	Spain	Male	Department of Materials Science and Physical Chemistry
Giménez Ortega	Xavier	Spain	Male	Department of Materials Science and Physical Chemistry
Huarte Larrañaga	Fermín	Spain	Male	Department of Materials Science and Physical Chemistry
López Marne	Estefanía	Spain	Female	Department of Materials Science and Physical Chemistry

Mota Valeri	Fernando	Spain	Male	Department of Materials Science and Physical Chemistry
Villacaña Pérez	Oscar	Spain	Male	Department of Materials Science and Physical Chemistry

ICREA Research Professors

Surname	Name	Country	Gender	Depart. Unit
Bromley	Stefan		Male	Department of Materials Science and Physical Chemistry
Neyman	Konstantin M.	Germany	Male	Department of Materials Science and Physical Chemistry
Poater Teixidor	Jordi	Spain	Male	Department of Inorganic and Organic Chemistry
Puigmartí Luis	Josep	Spain	Male	Department of Materials Science and Physical Chemistry
Rovira Virgili	Carme	Spain	Female	Department of Inorganic and Organic Chemistry

Lecturer Professors

Surname	Name	Country	Gender	Depart. Unit
Cortijos Aragonès	Albert	Spain	Male	Department of Materials Science and Physical Chemistry
Estarellas Martín	Carolina	Spain	Female	Department of Nutrition, Food Sciences and Gastronomy Basic Sciences Applied to Food Science
Gómez Coca	Silvia	Spain	Female	Department of Inorganic and Organic Chemistry
Jover Modrego	Jesús	Spain	Male	Department of Inorganic and Organic Chemistry
Juárez Jiménez	Jordi	Spain	Male	Department of Pharmacy and Pharmaceutical Technology, and Physical Chemistry
Morales García	Ángel	Spain	Male	Department of Materials Science and Physical Chemistry
Sorrenti	Alessandro	Italy	Male	Department of Inorganic and Organic Chemistry

Other Professors

Surname	Name	Country	Gender	Depart. Unit
Giménez Font	Xavier	Spain	Male	Department of Materials Science and Physical Chemistry
Llunell Marí	Miquel	Spain	Male	Department of Materials Science and Physical Chemistry

Lucas Alcorta	Josep Maria	Spain	Male	Department of Materials Science and Physical Chemistry
Ribeiro Moreira	Iberio de Piknho		Male	Department of Materials Science and Physical Chemistry
Solé Sabaté	Albert	Spain	Male	Department of Materials Science and Physical Chemistry
Vázquez Praga	David	Spain	Male	Department of Materials Science and Physical Chemistry
Vilaseca Font	Eduard	Spain	Male	Department of Materials Science and Physical Chemistry

Postdoctoral Researchers

Contracte Projecte de Recerca

Surname	Name	Country	Gender	Depart. Unit
Corbella Morató	Marina	Spain	Female	Department of Inorganic and Organic Chemistry
Garcia Cirera	Beltzane	Spain	Female	Department of Materials Science and Physical Chemistry
Kapse	Samadhan	India	Male	Department of Materials Science and Physical Chemistry
Nicholas	James	United Kingdom	Male	Department of Materials Science and Physical Chemistry
Rodríguez Remesal	Elena	Spain	Female	Department of Materials Science and Physical Chemistry
Stasyuk	Anton	Russia	Male	Department of Pharmacy and Pharmaceutical Technology, and Physical Chemistry
Voccia	Maria	Italy	Female	Department of Materials Science and Physical Chemistry

Ramón y Cajal

Surname	Name	Country	Gender	Depart. Unit
Bruix Fusté	Albert	Spain	Male	Department of Materials Science and Physical Chemistry
Cirera Fernández	Jordi	Spain	Male	Department of Inorganic and Organic Chemistry
Fumanal Quintana	Maria	Spain	Female	Department of Materials Science and Physical Chemistry
Guix Noguera	Maria	Spain	Female	Department of Materials Science and Physical Chemistry
Kumar	Mohit	India	Male	Department of Inorganic and Organic Chemistry
Matheu	Roc	Spain	Male	Department of Inorganic

				and Organic Chemistry
Raich	Lluís		Male	Department of Inorganic and Organic Chemistry

Beatriu de Pinós-Juan de la Cierva

Surname	Name	Country	Gender	Depart. Unit
Boukinala	Moses Abraham	India	Male	Department of Materials Science and Physical Chemistry
Vela Llausí	Sergi	Spain	Male	Department of Materials Science and Physical Chemistry

Marie-Curie

Surname	Name	Country	Gender	Depart. Unit
Liao	Qinghua	China	Male	Department of Inorganic and Organic Chemistry

Maria de Maeztu

Surname	Name	Country	Gender	Depart. Unit
Evans	Rhys	United Kingdom	Male	Department of Nutrition, Food Sciences and Gastronomy Basic Sciences Applied to Food Science

Others

Surname	Name	Country	Gender	Depart. Unit
Baraorda-Ccahuana	Haruna			Department of Materials Science and Physical Chemistry
Blanco Andrés	Pablo	Spain	Male	Department of Materials Science and Physical Chemistry
Calvelo Souto	Martin		Male	Department of Inorganic and Organic Chemistry
Llabrés Prat	Salomé	Spain	Female	Department of Nutrition, Food Sciences and Gastronomy Basic Sciences Applied to Food Science
Mattera	Michele		Male	Department of Materials Science and Physical Chemistry
Noori	Zhars	Spain	Female	Department of Inorganic and Organic Chemistry
Saletra	Wojciech		Male	Department of Inorganic and Organic Chemistry
Saranjam	Leila			Department of Materials Science and Physical Chemistry

Predoctoral Researchers

FI Grant

Surname	Name	Country	Gender	Depart. Unit
Betkhoshvili	Sergi	Georgia	Male	Department of Inorganic and Organic Chemistry
Blanco Gabella	Patricia	Spain	Female	Department of Pharmacy and Pharmaceutical Technology, and Physical Chemistry
Dolz García	Daniel	Spain	Male	Department of Materials Science and Physical Chemistry
García-Romeral González	Néstor Mauricio	Spain	Male	Department of Materials Science and Physical Chemistry
Llauradó Capdevila	Gemma	Spain	Female	Department of Materials Science and Physical Chemistry
Mariñoso Guiu	Joan		Male	Department of Materials Science and Physical Chemistry
Özaydin	Gül Beste	Turkey	Female	Department of Pharmacy and Pharmaceutical Technology, and Physical Chemistry
Piniello Castillo	Beatriz	Spain	Female	Department of Inorganic and Organic Chemistry
Vila Julia	Guillem		Male	Department of Materials Science and Physical Chemistry

FPI Grant

Surname	Name	Country	Gender	Depart. Unit
Allès Coll	Miquel	Spain	Male	Department of Materials Science and Physical Chemistry
Almacellas Salillas	David	Spain	Male	Department of Inorganic and Organic Chemistry
Calzada Escrig	Adrià	Spain	Male	Department of Materials Science and Physical Chemistry
Cánovas Montes	Manuel Antonio	Spain	Male	Department of Materials Science and Physical Chemistry
Castro Latorre	Pablo	Chile	Male	Department of Materials Science and Physical Chemistry
Cortés Llamas	Arnau	Spain	Male	Department of Materials Science and Physical Chemistry
Cuxart Sánchez	Irene	Spain	Female	Department of Inorganic and Organic Chemistry
Farris	Riccardo	Italia	Male	Department of Materials Science and Physical Chemistry
Gómez Silvestre	Francisco Alonso	Spain	Male	Department of Inorganic and Organic Chemistry

Mamusi	Fatemeh	Spain	Female	Department of Materials Science and Physical Chemistry
Recio Poo	Miguel	Spain	Male	Department of Materials Science and Physical Chemistry
Regalado Aguilar	Mauricio	Spain	Male	Department of Inorganic and Organic Chemistry
Rivas Fernández	José Pablo	Spain	Male	Department of Inorganic and Organic Chemistry
Romeo	Eleonora	Italy	Female	Department of Materials Science and Physical Chemistry
Silvestre Llora	Adriana	Spain	Female	Department of Inorganic and Organic Chemistry
Vidal Gironès	Òscar	Spain	Male	Department of Inorganic and Organic Chemistry

FPU Grant

Surname	Name	Country	Gender	Depart. Unit
Lozano Reis	Pablo	Spain	Male	Department of Materials Science and Physical Chemistry
Orradre Altabás	Javier	Spain	Male	Department of Materials Science and Physical Chemistry

ITN UE Grant

Surname	Name	Country	Gender	Depart. Unit
Ergün	Özge	Turkey	Female	Department of Pharmacy and Pharmaceutical Technology, and Physical Chemistry

UB/ADR Grant

Surname	Name	Country	Gender	Depart. Unit
Dias da Cunha	Renato	Brazil	Male	Department of Pharmacy and Pharmaceutical Technology, and Physical Chemistry
Jutglar Lozano	Kílian	Spain	Male	Department of Materials Science and Physical Chemistry
López Berbel	Martí	Spain	Male	Department of Materials Science and Physical Chemistry
Martínez Medina	Yaiza	Spain	Female	Department of Inorganic and Organic Chemistry
Peralta Moreno	Maria Nuria	Spain	Female	Department of Materials Science and Physical Chemistry

Contracte Projecte de Recerca

Surname	Name	Country	Gender	Depart. Unit
Díaz Canals	Blanca	Spain	Female	Department of Pharmacy and Pharmaceutical Technology, and Physical Chemistry
Gonzalo Palao	Daniel	Spain	Male	Department of Pharmacy and Pharmaceutical Technology, and Physical Chemistry

J. E. Delima	David	Philippines	Male	Department of Inorganic and Organic Chemistry
Pepe	Alessandro	Italia	Male	Department of Inorganic and Organic Chemistry
Sağıroğlugil	Mert	Turkey	Male	Department of Inorganic and Organic Chemistry

Contracte Maria de Maeztu

Surname	Name	Country	Gender	Depart. Unit
Colomer Llombart	Eduard	Spain	Male	Department of Materials Science and Physical Chemistry
Gracia Gil	Alejandro	Spain	Male	Department of Materials Science and Physical Chemistry

Others

Surname	Name	Country	Gender	Depart. Unit
Alsina Cowie	Marc	Spain	Male	Department of Inorganic and Organic Chemistry
Barmpidi	Katerina	Greece	Female	Department of Nutrition, Food Sciences and Gastronomy Basic Sciences Applied to Food Science
Blas Buch	Daniel	Spain	Male	Department of Materials Science and Physical Chemistry
Cabello Gallego	Ruben	Spain	Male	Department of Chemical Engineering and Analytical Chemistry
Cao	Wei	China	Male	Department of Materials Science and Physical Chemistry
De Donato Pérez	Andreu Avel·lí	Spain	Male	Department of Materials Science and Physical Chemistry
De Moya Valenzuela	Natalia	Spain	Female	Department of Materials Science and Physical Chemistry
Distefano	Chiara	Italy	Female	Department of Inorganic and Organic Chemistry
Esquivias Bautista de Lisbona	Oriol		Male	Department of Inorganic and Organic Chemistry
Garcia Gonzalo	Lluc	Spain	Male	Department of Inorganic and Organic Chemistry
Gómez Gordo	Mireia	Spain	Female	Department of Nutrition, Food Sciences and Gastronomy Basic Sciences Applied to Food Science
Herrera Restrepo	Ramón Santiago	Colombia	Male	Department of Materials Science and Physical Chemistry
Ivanova	Varbina		Female	Department of Pharmacy and Pharmaceutical Technology,

				and Physical Chemistry
Jurado Mañas	Anabel	Spain	Female	Department of Materials Science and Physical Chemistry
Lleopart Motis	Genís		Male	Department of Materials Science and Physical Chemistry
Martí Sanz	Mir	Spain	Male	Department of Inorganic and Organic Chemistry
Meng	Ling	China	Female	Department of Materials Science and Physical Chemistry
Morales Salvador	Raúl	Spain	Male	Department of Materials Science and Physical Chemistry
Navarro Maestro	Laia	Spain	Female	Department of Inorganic and Organic Chemistry
Ngo	Tuan	Vietnam	Male	Department of Materials Science and Physical Chemistry
Nguyen	Thao	Vietnam	Female	Department of Materials Science and Physical Chemistry
Ontiveros Cruz	Diego	Spain	Male	Department of Materials Science and Physical Chemistry
Quinlinvan Domínguez	Jon Eunan	Spain	Male	Department of Materials Science and Physical Chemistry
Santiago Piera	Raúl	Spain	Male	Department of Materials Science and Physical Chemistry
Serrano Morrás	Álvaro	Spain	Male	Department of Pharmacy and Pharmaceutical Technology, and Physical Chemistry
Troyano Ferré	Carles	Spain	Male	Department of Chemical Engineering and Analytical Chemistry
Valdivia Escribà	Aitor	Spain	Male	Department of Nutrition, Food Sciences and Gastronomy Basic Sciences Applied to Food Science
Vanrell Sabater	Antoni	Spain	Male	Department of Inorganic and Organic Chemistry
Vidal Ramón	Daniel	Spain	Male	Department of Materials Science and Physical Chemistry

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*
Begoña López Maestre	*Project Manager*
Patricia Verdugo Salomón	*3D Designer*
Aïda Valverde Sanchís	*Project Manager and Promoter*

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

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

lqtc10 (*invested value 164.000 €*)

Machine type Gigabyte Cluster
Operating System Centos 7.2
Services Calculation cluster
Structure 9 nodes (32 GPU RTX 3090, 8 RTX3080)
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

3 Gigabyte G292-Z44-00
CPU: 2 x 2.8 GHz AMD EPYC 7282 16-core processor (32 cores)
RAM: 256 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

1 Gigabyte G482-Z54-00
CPU: 2 x 2.8 GHz AMD EPYC 7282 16-core processor (32 cores)
RAM: 256 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: 8 x RTX3080 NVIDIA

Iqtc11 (*invested value 100.000 €*)

Machine type	Gigabyte Cluster
Operating System	Centos 7.2
Services	Calculation cluster
Structure	9 nodes + 1 file server
Notes	64 bits processors

Specifications

9 Gigabyte R182-340-00
CPU: 2 x 2.80GHz Intel Xen Plantium 8362 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

1 Gigabyte R282-3C1-00
CPU: 2 x 2.60Ghz Intel Xen Plantium 8358 32-core processor (64 cores)
RAM: 128 GB
HD: 100 TB SATA hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (internal administration network) + 2 x 10 GB network card

GPU cluster (*invested value 75.000 €*)

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

Specifications:

Node
CPU: 1 x 3,06 GHz Intel Core i7 950

RAM: 16 GB
HD: 1 x 1 TB hard disk
Network: 1 gigabit network card (calculation network)
GPU: 1 NVIDIA GTX580, 1 NVIDIA GTX480

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

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

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

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

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

Node SIE LADON BROADWELL
CPU: 2 x 2,4 GHz Xeon E5-2640v4
RAM: 128 GB
HD: 1 x 1 TB hard disk

Network: 2 gigabit network card (calculation network) + 1 IPMI card (OOB)
GPU: 4 NVIDIA TESLA K40

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

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

Servers

Disk server (*invested value 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. 6 Oculus Quest

The approximated invested cost of this equipment is *58.000 €.*

Summary

Cores .....5,972 c

Memory.....82,276 GB RAM

Calculation disk capacity..... 263 TB

Data user disk capacity..... 75 TB

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

*2.000.000 €**

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

IQTCUB ACTIVITIES

General Activities (courses, grants and dissemination)

Next, a description of activities and actions promoted by IQTCUB through 2023 is provided.

a. ***Molecular Modelling: biomolecules and drug design 2023.*** From February 7th to 10st, the summer computational school titled *Molecular Modelling: biomolecules and drug design 2023 took place.* Prof. Sergio Madurga and Prof. Jaime Rubio organized the event. In this edition, the sessions were given by the following researchers:

- Analysis of non-covalent interactions in DNA base pairs. (Jordi Poater)

- Simulation of macromolecular systems (Sergio Madurga)

- Protein Molecular Dynamics (Carolina Estarellas and Salomé Llabrés)

- Visualising biomolecules in action (Matín Calvelo and José Pablo Rivas)

- Coarse-grained Molecular Dynamics simulations for soft-matter systems: from micelles to membranes (Ramón Reigada)

- Drug Design (Jaime Rubio)

- Multi-scale modelling of solutions and biomolecules (Carles Curutchet)

b. Computational Modelling: from Molecules to Materials 2023. From February 13th to 17th, the summer computational school titled *Computational Modelling: from Molecules to Materials 2023* took place. The organizers were Dr. Silvia Gómez and Prof. Gabriel Aullón. In this edition, the sessions were given by the following researchers:

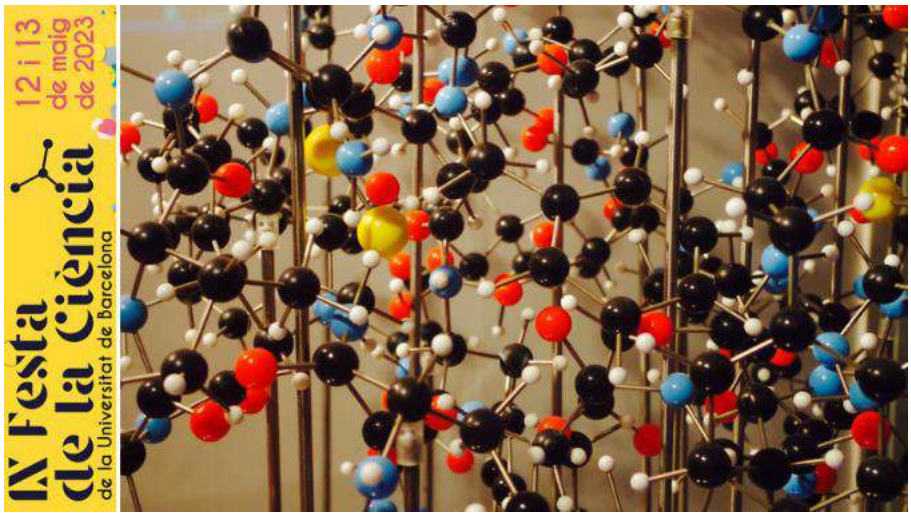
- Linux (Jordi Inglés and Irene Zamora)
- Linkage and structure (Gabriel Aullón and Silvia Gómez)
- Excited States (Mercè Deumal)
- Molecular Reactivity (Jesús Jover)
- Molecular dynamics (Miguel González)
- Virtual reality in chemistry (Jordi Cirera)
- Nanoclusters and Nanostructures Materials (Stefan Bromley)
- Band Theory (Eliseo Ruiz)
- Surfaces and defects (Ángel Morales)
- Machine Learning (Albert Bruix)

c. ***Cafè amb Científiques.*** The event took place on February 17th 2023. The discussion was carried out by the following speakers:

- Irene Ferri Condeminas: predoc researcher (UBICS)
- Dr. Alba Espargaró Colomé: Lector professor (IN2UB)
- Maria Guix: Ramón y Cajal researcher (IQTC)
- Dr. Núria López Vinent: Margarita salas postdoc (IDRA)
- Júlia Molins i Vigatà: PhD student (Institute of Geomodels)
- Ana Climent: PhD student (ICCUB)
- Dr. Maria Elena Xuriguera: associate professor (DIOPMA)
- Creu Palacín Cabañas: full professor (IRBIO)

d. ***Minisymposium IN²UB-IQTCUB***. The minisymposium co-organized with the IN²UB on Spectroscopic Trends for Quantum Technologies and Spintronics with Magnetic Molecules took place on March 22nd 2023. The talkers in this seminar were Dr. Matteo Atzori and Prof. Joris van Slageren.

e. ***IX Festa de la Ciència.*** The IQTC paticipated with the "Explora el món molecular en un entorn de realitat virtual" workshop. It took place on May 12th and 13th.



f. ***IQTCUB Meeting 2023.*** The event took place on September 18th and 19th. The workshop allowed the IQTC members to share the findings obtained from their research. The aim of the event was to broaden the views on topics of interest to the community. Some international researchers talked at this seminar, like Dr. Michael Robb from Imperial College and Dr. Pierre-Francois Loos from the Université de Toulouse. A poster session was held as well for this event.

g. ***New Trends in Computational Chemistry 2023.*** This workshop was held on September 19th and 20th and it brought together worldwide leading experts in the application and development of Quantum Computing methods applied to virtual reality like Dr. David Glowacki and Dr. Mel Slater and companies like Nanome, Immersium Studio and Digivision.

IQTCUB Seminars and Conferences

During 2023 IQTC has organized the following seminars and conferences:

Dr. Juan José Nogueira (MoBioChem Research Group, Universidad Autónoma de Madrid)
Effect of Solvent and Biological Environments on Electronic Structure Properties.
January 11th 2023

Prof. Roald Hoffmann (Cornell University)
All the Ways to have a Bond
January 24th 2023

Dr. Brigit Strodel (Computational Biochemistry Group, Forchungszentrum Jülich)
From QM/MM to MD Simulations and Machine-Learning for the Redesign of PETases and Esterases
February 8th 2023

Dr. Biel Martínez (Comissaritat à l'Énergie Atomique Grenobele)
The stumbling blocks of a large-scale spin qubit quantum computer
April 20th 2023

Prof. Dario Estrín (University of Buenos Aires, Argenitna)
QM/MM studies of Fe-reactivity process involved in hemoglobulins: towards understanding foundations of survival mechanism of bacterial.
May 5th 2023

Prof. Jayant K. Singh (Department of Chemical Engineering, Indian Institute of Technology)
Insight into the ice formation at extreme confinement and under shear flow
May 26th 2023

Dr. Isaac Alcón (Institut Català de Nanociència i Nanotecnologia)
Engineering of Charge Current Flow in Nanoporous Graphenes
June 22nd 2023

Dr. Teodoro Laino (IBM Research Europe)
Fueling the Digital Chemistry Revolution with Language Models
June 30th 2023

Prof. Louise Serpell (University of Sussex, UK)
Untangling the misfolding proteins in Alzheimer's disease.
July 17th 2023

Silke Rimaux (University of KU Leuven, Belgium)
Pseudovirus entry and cell-cell fusion assays: Two biological methods to study influenza virus hemagglutinin and its inhibitors
September 21st 2023

Prof. Fernando Martín (Universidad Autónoma de Madrid, IMDEA-Nano)
Real-time imaging and control of electron dynamics in molecules: towards attosecond chemistry
November 7th 2023

Prof. Alberto Roldán (Cardiff Catalysis Institute, Cardiff University)
Advances in the Rational Approach for Modelling Supported Catalysts
November 21st 2023

Dr. Max García-Melchor (School of Chemistry, Trinity College)
Rational Design of Catalytic Materials for Energy Conversion
December 19th 2023

IQTCUB Invited Researchers

Dr. Juan José Nogueira (invited visitor)
Autonomous University of Madrid, Spain
January 2023

MSc. Alexander Robertson (invited visitor)
University of York, United Kingdom
January 2023 (three weeks)

Prof. Samanta Makurat (invited visitor)
University of Gdansk, Poland
January 2023 (one month)

MSc. Giacomo Salvatori (invited visitor)
University of Pisa, Italy
February 2023 to May 2023

Dr. José Hernández (visiting professor with a Coimbra Group grant)
Universidad de Antioquia, Colombia
April-May 2023

Prof. Paula Homem de Mello (invited visitor)
Federal University of ABC, Brazil
May-July 2023

MSc. Ignacio Jesús Sanz (invited visitor)
University of Zaragoza, Spain
May 2023 - July 2023

Prof. Mariana Morais (invited visitor)
CNPEM-Brazil, Brazil
June 2023 (three weeks)

Prof. Hristiyan A. Aleksandrov (invited visitor)
University of Sofia, Bulgaria
July 2023

M. Sc. Stoyan Gramatikov (invited visitor)
University of Sofia, Bulgaria
July 2023

Prof. Jaakko Akola (invited visitor)
Norwegian University of Science and Technology - NTNU, Norway
August 2023 - June 2024

Ms. Anna Jelinková (invited visitor)
Palacký University Olomouc, Czech Republic
September-December 2023

Prof. Michael A Robb (invited visitor)
Imperial College London, United Kingdom
September 2023

Prof. Petr Jurečka (invited visitor)
Palacký University Olomouc, Czech Republic
October 2023

Prof. Marie Zgarbová (invited visitor)
Palacký University Olomouc, Czech Republic
October 2023

PhD student Somia Benchikh (invited visitor)
Ferhat Abbas University of Setif, Algeria
October-November 2023

MSc. Carlos Álvarez (invited visitor)
Norwegian University of Science and Technology - NTNU, Norway
October 2023 - November 2023

Federico Crocci (Laurea student)
University degli Studi di Perugia (Italy)
February 2023 to September 2023

Alessandro Galadeta (Laurea student)
University degli Studi di Bari (Italy)
February 2023 to September 2023

Valentin Rech (Master student)
Julius Maximilian University Wurzburg (Germany)
October 2023 to February 2024

Francesca Procopio (Laurea student)
Università degli Studi di Catanzzaro (Italy)
February 2023 to July 2023

Fajar Puteras (Erasmus Master student)
University of Algarve (Portugal)
February 2023 to September 2023

Prof. Dr. Guadalupe Moreno (invited visitor)
Universidad Nacional Autónoma de México, México
January to December 2023

Prof. Professor Jianhua Hou (invited visitor, CSC programme)
Changchun University of Science and Technology, Changchun, P. R. China
October 2023 to September 2024

Mrs. Tahereh Tahereh Jangjooye Shaldehi
Iran University of Science and Technology, Iran
February to September 2023

Scientific Activity of IQTCUB Members
Highlights from most Relevant Results

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

Line 1. Catalysis, energy, and environment

States of Pt/CeO_2 catalysts for CO oxidation below room temperature.
E.M. Slavinskaya, A.I. Stadnichenko, J.E. Quinlivan Domínguez, O.A. Stonkus, M. Vorokhta, B. Šmíd, P. Castro-Latorre, A. Bruix, K.M. Neyman, A.I. Boronin.
J. Catal., *421* (2023) 285-299.

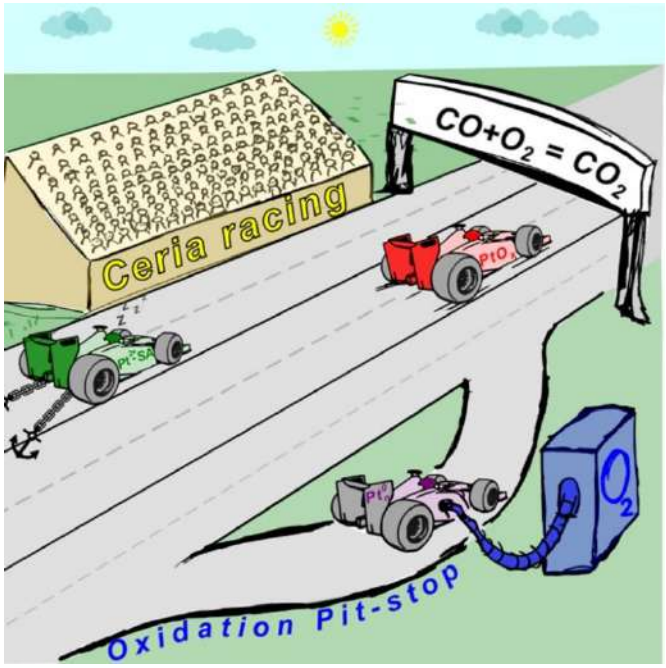


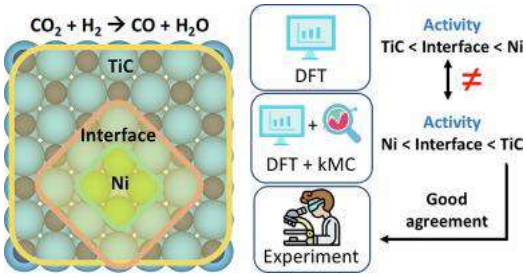
Figure. The red car wins: small PtO_x oxide clusters enable oxidation of poisonous exhaust CO molecules to CO_2 at abnormally low temperatures (courtesy of Dr. A. Stadnichenko).

Noble metal platinum becomes not-noble at the nanoscale. Platinum is a precious metal remarkably resistant to oxidation and corrosion. It is one of the most noble metals widely used in technology. Bulk Pt is not oxidized by oxygen in air at any temperature and a very thin surface platinum oxide layer is unstable and easily removable by heating.
Is such high resistivity to oxidation observed in the macro-world also characteristic of Pt in the micro-world, when the size of platinum particles decreases to the nanometre scale? This question is particularly relevant for catalytic applications, in which Pt is indispensable component as nanometre-size particles deposited on oxide supports. Such Pt_n particles are considered at moderate oxygen pressure and temperatures as metallic, i.e. not containing oxygen. Research team of Konstantin Neyman and Albert Bruix performed quantum-mechanical simulations of the stability of small Pt_nO_m particles, with $n \leq 6$ Pt atoms, $m \leq 2n$. Surprisingly, it was calculated that even at low O_2 pressure of 0.01 atm and room temperature both free and oxide-supported particles are most stable in significantly oxidised states PtOx, where all Pt-Pt bonds were transformed into Pt-O-Pt bonds. These findings revealing dramatic changes of noble metal platinum to become easily oxidised at the nanoscale resulted from international collaboration with an experimental group that prepared supported on ceria (CeO_2) Pt catalysts efficient for oxidation of poisonous carbon monoxide molecules at abnormally low temperatures, beneficial for air pollution abatement. Interestingly (see figure), such low-temperature CO abatement is triggered by the oxidised PtOx species, co-existing species containing other ionic forms of Pt atoms acting to oxidise CO at higher temperatures and still present metallic Pt_n species undergoing oxidation.

Sustainable Use of Energy Contributes to Carbon Neutrality and Environmental Footprints Reduction
Wang, X.-C., Wang, J., Plesu Popescu, A.E., Yang Ong, B.H.
Energy 285 (2023) 129464.

Alexandra Plesu as a member of the International Scientific Committee of the Conference on Process Integration, Modelling and Optimization for Energy Saving and Pollution Reduction (PRES), among the different duties developed in this framework of the conference has been assigned the role of reviewer of the selected papers for an special issue of the Energy journal focused on improving the sustainable use rate of energy and contribute to carbon neutrality and environmental footprints reduction.

Limitations of free energy diagrams to predict the catalytic activity: The reverse water gas shift reaction catalyzed by Ni/TiC
Lozano-Reis, P., Prats, H., Sayós, R., Illas, F.
Journal of Catalysis 425 (2023) 203-211.



The temporal evolution at the catalyst surface is a result of an intricate interplay between all involved microscopic events such as adsorption, desorption, diffusion, and bond breaking/formation steps, and the interaction with the surrounding environment. By properly including these effects, kinetic Monte Carlo (kMC) simulations can accurately describe the complexity of real catalysts, unravel the dominant reaction mechanisms and provide fundamental understanding towards the rational design of novel catalysts. In this work, we combine density functional theory (DFT) calculations, statistical thermodynamics and kMC simulations to study the reverse water–gas shift (RWGS) reaction on Ni/TiC, a bifunctional catalyst. The predictions from DFT energy profiles do not coincide with the outcome of the kMC simulations, evidencing the limitations of the former, especially in including the effect of coverage of surface species.

Potential energy surfaces for singlet and triplet states of the LiH_2^+ system and quasi-classical trajectory cross sections for H + LiH^+ and H^+ + LiH
J. Hernández-Rodríguez, C. Sanz-Sanz, P. A. Enríquez, M González, M. Paniagua
Phys. Chem. Chem. Phys., *25* (2023) 28052.

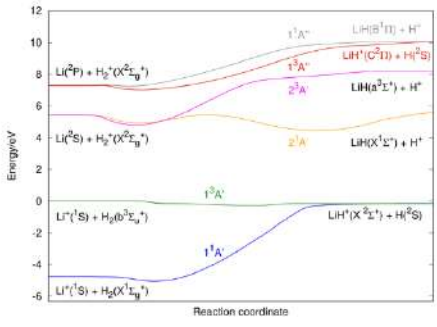
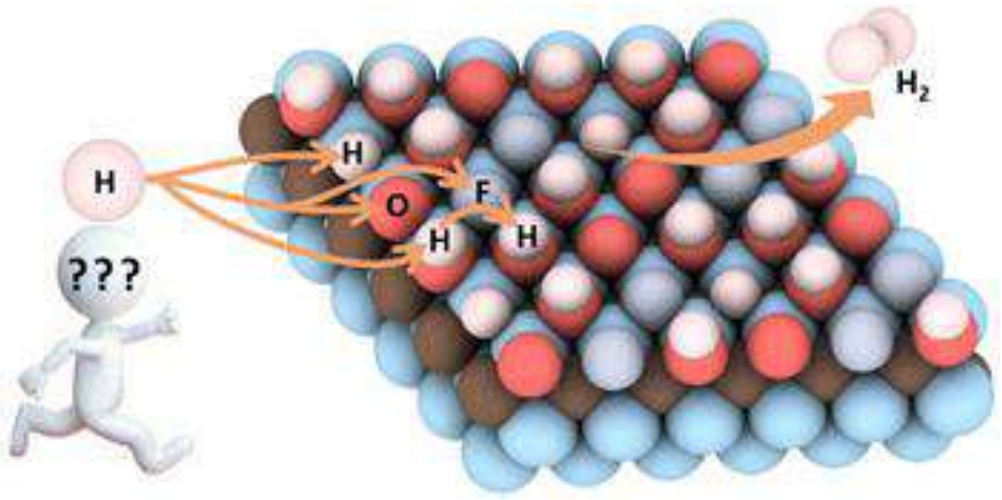


Figure. Schematic representation of the minimum energy paths connecting the $Li^+ + H_2$ and $Li + H_2^+$ reactants with the $LiH^+ + H$ and $LiH + H^+$ products, respectively (except for the $1^3A''$ potential energy surface, where $Li + H_2^+$ connects with $LiH^+ + H$).

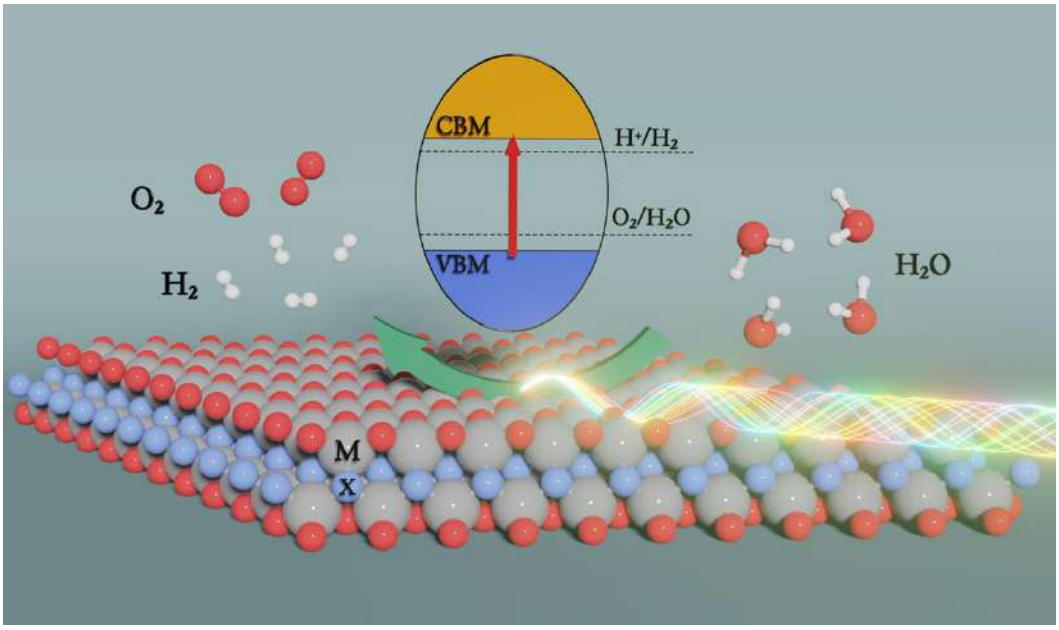
Six accurate ab initio potential energy surfaces (PESs) are presented for the first three singlet and triplet states of LiH_2^+ (1,2 ^{1}A', 1 ^{1}A'', 1,2 ^{3}A' and 1 ^{3}A'' states), where four of them are investigated for the first time. This has allowed new detailed studies gaining a global view on this interesting system. These states are relevant for the study of the most important reactions of lithium chemistry in the early universe. More than 45000 energy points were calculated using the multi-reference configuration interaction level of theory using explicitly correlated methods (ic-MRCI-F12), and the results obtained for each individual electronic state were fitted to an analytical function. Using quasiclassical trajectories and considering the initial diatomic fragment in the ground rovibrational state, we have determined the integral cross sections for the H + LiH+($X^2\Sigma^+$, $C^2\Pi$) and H+ + LiH($X^1\Sigma^+$, $B^1\Pi$) reactions. In these calculations all available reaction channels were considered: the chemically most important H or H^+ transfer/abstraction as well as atom
exchange and collision induced dissociation, for up to 1.0 eV of collision energy. To the best of our knowledge this is the reactive system for which more electronic states have been studied simultaneously and the corresponding analytic expressions of the PESs have been reported.

Effect of Terminations on the Hydrogen Evolution Reaction Mechanism on Ti_3C_2 MXene.
L. Meng, L.-K. Yan, F. Viñes, F. Illas.
J. Mater. Chem. A., *11* (2023) 6886.



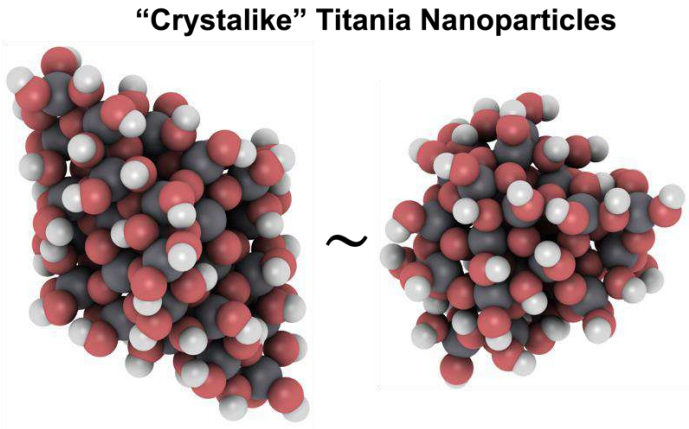
Two-dimensional (2D) MXene materials are proposed as high-efficiency hydrogen evolution reaction (HER) electrocatalysts. Most computational studies addressed the HER assuming a fully O-termination, even if as-synthesized MXenes feature a mixture of –O, –OH, –F, or even –H surface groups. To better understand the electrocatalytic surface composition and mechanism under HER equilibrium conditions in the Ti3C2 MXene model material, we composed Pourbaix diagrams considering ca. 450 topologically different surface terminations, including pristine Ti3C2, full –O, –OH, –F, and –H terminations, and binary and ternary situations with different group ratios. Realistic models built from Pourbaix diagrams near HER equilibrium conditions of low pH and U were used to investigate the Volmer–Heyrovsky and Volmer–Tafel mechanisms, with the particularity of considering, or not, the participation of H atoms from –OH or –H termination groups at different reaction stages. Results pointed out that the models close to the HER equilibrium line, O2/3OH1/3, F1/3O1/3OH1/3, and F3/9O4/9OH2/9, require an almost negligible overpotential of 0.01 V, while surface charges explain the impact of higher ratios of –O groups on modulating the H bond, and the positive influence of having surface –F groups.

Bandgap engineering of MXene compounds for water splitting.
D. Ontiveros, F. Viñes, C. Sousa.
J. Mater. Chem. A., *11* (2023) 13754-13764.



A recently discovered family of 2D MXenes materials have been found to become semiconductors and photoactive when their pristine surfaces are functionalized with an electronegative termination. MXenes may present different compositions and structures, depending on the transition metal (M= Sc, Y, Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, W), the X-element (C or N), the stacking and termination site. Here, we performed DFT calculations to engineer the bandgap of a wide range of MXenes by their structure, composition, and surface termination with oxygen, in order to find suitable materials for water splitting photocatalysis. Results showed that pristine MXenes present metallic character in all cases, while adding the O-termination increases the chance of becoming a semiconductor. Group III and IV MXenes turn out to be the most promising bandgap systems for photocatalysis. Concerning the X element, C-MXenes exhibit more cases with bandgap than N-MXenes, and generally with larger values. For all the cases presenting a bandgap larger than 1.23 eV, the minimum demanded for the water splitting process, the band alignment with respect the water splitting half-reactions potentials was studied, obtaining Zr_2CO_2 as a promising photocatalysts for this process.

Crystal properties without crystallinity? Influence of surface hydroxylation on the structure and properties of small TiO_2 nanoparticles.
M. Recio-Poo, Á. Morales-Garcia, F. Illas, S. T. Bromley.
Nanoscale, *15* (2023) 4809-4820.



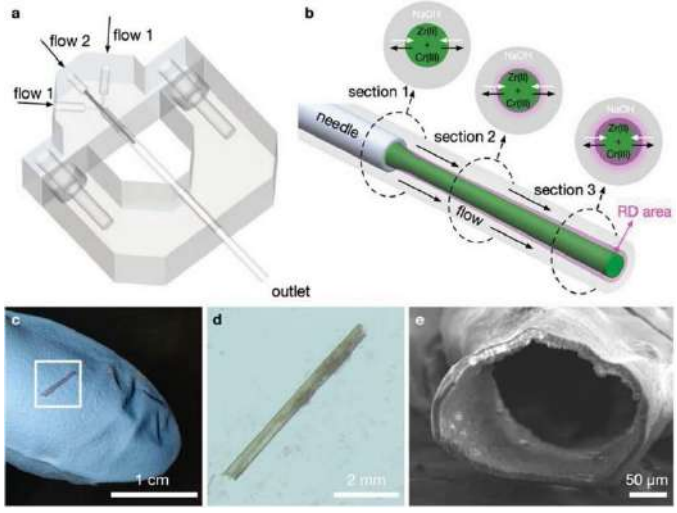
Titania (TiO_2) nanoparticles (NPs) are widely employed in applications that take advantage of their photochemical properties (*e.g.* pollutant degradation, photocatalysis). Here, we study the interrelation between crystallinity, surface hydroxylation and electronic structure in titania NPs with 1.4–2.3 nm diameters using all electron density functional theory-based calculations. We show how the distribution of local coordination environments of the atoms in thermally annealed quasi-spherical non-crystalline NPs converge to those in correspondingly sized faceted crystalline anatase NPs upon increasing hydroxylation. When highly hydroxylated, annealed NPs also possess electronic energy gaps with very similar energies and band edge orbital characters to those of the crystalline anatase NPs. We refer to the crystallite-mimicking non-crystalline annealed NPs as "crystalikes". Small stable crystalike NPs could allow for photochemical applications of titania in the size range where crystalline anatase NPs tend to become thermodynamically unfavoured (<3–5 nm). Our work implies the anatase crystal structure may not be as essential as previously assumed for TiO_2 NP applications and generally suggests that crystalikes could be possible in other nanomaterials.

Line 2. Nanomaterials for emergent technologies

"On-The-Fly" Synthesis of Self-Supported LDH Hollow Structures Through Controlled Microfluidic Reaction-Diffusion Conditions

M. Mattera, A. Sorrenti, L. De Gregorio Perpiñá, V. Oestreicher, S. Sevim, O. Arteaga, X.-Z. Chen, S. Pané, G. Abellán, J. Puigmartí Luis.

Small., *20* (2023) 2307621.



Tailored Design of a Water-Based Nanoreactor Technology for Producing Processable Sub-40 Nm 3D COF Nanoparticles at Atmospheric Conditions

Gemma Llauradó-Capdevila, Andrea Veciana, Maria Aurora Guarducci, Alvaro Mayoral, Ramon Pons, Lukas Hertle, Hao Ye, Minmin Mao, Semih Sevim, David Rodríguez-San-Miguel, Alessandro Sorrenti, Bumjin Jang, Zuobin Wang, Xiang-Zhong Chen, Bradley J. Nelson, Roc Matheu, Carlos Franco, Salvador Pané, Josep Puigmartí-Luis

Adv. Mater., 2023, 2306345.

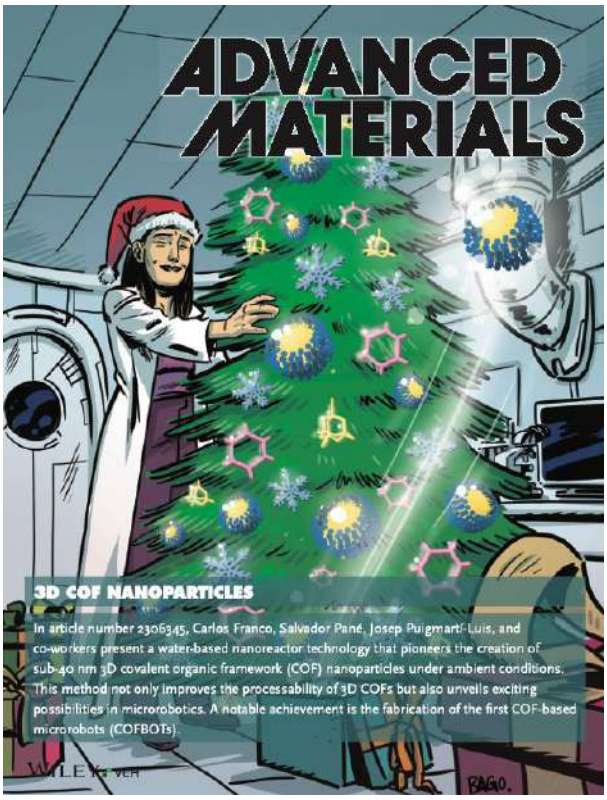


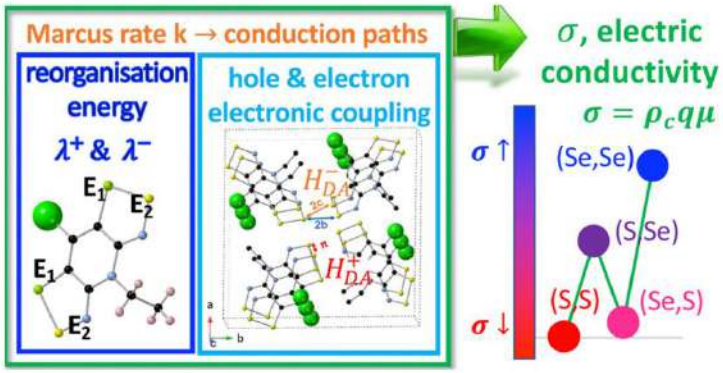
Figure. Advanced Materials selected our cover design suggestion to be featured on a frontispiece in the issue.

Covalent organic frameworks (COFs) are crystalline porous materials that offer a wide range of potential applications spanning diverse fields. Yet, the main goal in the COF research area is to achieve the most stable product while simultaneously targeting the desired size and structure crucial for enabling specific functions. While significant progress is made in the synthesis and processing of 2D COFs, the development of processable 3D COF nanocrystals remains challenging. Here, a water-based nanoreactor technology for producing processable sub-40 nm 3D COF nanoparticles at ambient conditions is presented. Significantly, this technology not only improves the processability of the synthesized 3D COF, but also unveils exciting possibilities for their utilization in previously unexplored domains, such as nano/microrobotics and biomedicine, which are limited by larger crystallites.

Understanding trends in conductivity in four isostructural multifunctional crystals of Se substituted bis-dithiazolyl radicals

C. Roncero-Barrero, M.A. Carvajal, J. Ribas-Ariño, I. de P.R. Moreira, M. Deumal.

J. Mater. Chem. C., *12* (2024) 468.



Materials based on stable organic radicals are very promising for the development of single-component organic conductors. However, the lack of studies addressing the quantitative calculation of the parameters defining their conductivity hampers progress. In this article, we have computationally studied four isostructural compounds with different Se-contents belonging to the key pyridine-bridged bisdithiazolyl family (namely, (S,S)-bisdithiazolyl, (S,Se) and (Se,S) mixed-thiaselenazolyl, and (Se,Se)-bisdiselenazolyl) with remarkable variation in the electrical conductivity ($\sigma_{SS} < \sigma_{SeS} < \sigma_{SSe} < \sigma_{SeSe}$) that cannot be explained on simple grounds. This trend can be explained by analyses of the local microscopic parameters playing the leading role in charge transport mediated by the molecular hopping mechanism: reorganization energy (λ), electronic couplings (H_{DA}), electron-transfer rate constants (k_{DA}), and charge-carrier density (ρ_c). Our results reveal the preference for hole conduction. The lowest conductivity of (S,S) arises from its largest λ, and smallest H_{DA}'s and ρ_c, resulting in a 1D conductor along the π-stack. Instead, the largest conductivity of (Se,Se) originates in its smallest λ, largest ρ_c and a set of H_{DA} electronic couplings that not only are the largest but also define a 3D topology of conduction pathways along both lateral contacts and π-stacking. Comparison of (Se,S) and (S,Se) shows that although (Se,S) features the largest k_{DA} and the smallest λ values, (S,Se) exhibits the largest electrical conductivity since it shows a 3D conduction topology because of lateral contacts and has a larger ρ_c value. Our calculations demonstrate that one needs to master a holistic view of the parameters governing the charge transport process (namely, λ, H_{DA}, topology of conduction paths, and ρ_c) to understand the trends in conductivity in radical-based molecular materials.

Line 3. Biocatalysis and drug discovery

Engineering excitonically coupled dimers in an artificial protein for light harvesting via computational modeling.
M. Curti, V. Maffeis, L.G. Teixeira Alves Duarte, S. Shareef, L.X. Hallado, C. Curutchet, E. Romero
Protein Sci. *32* (2023) e4579.

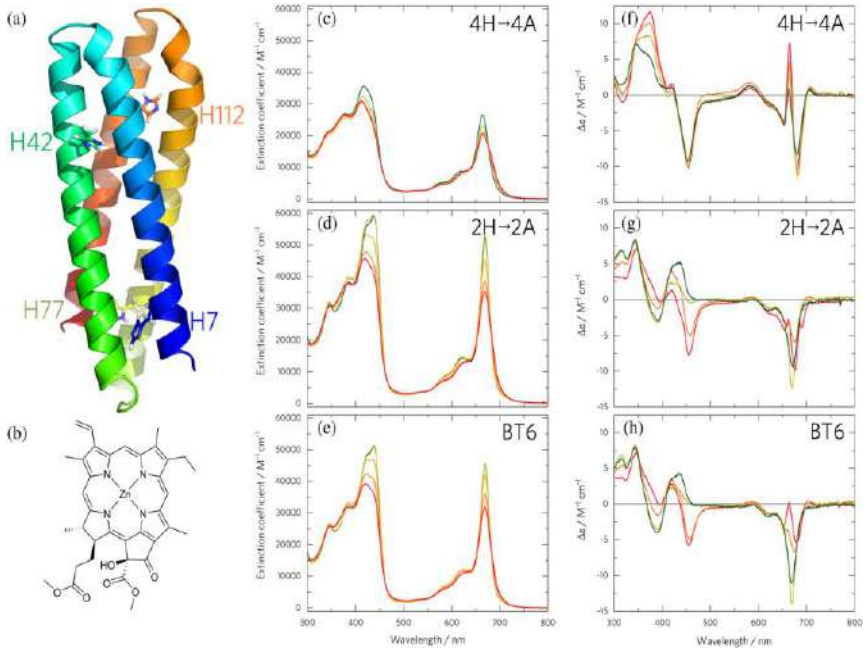
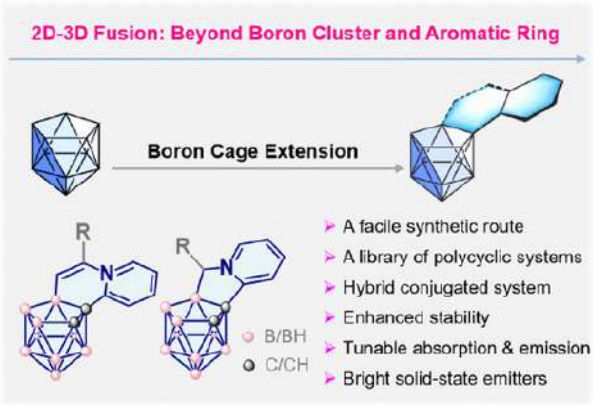


Figure. The artificial protein BT6 was engineered to incorporate an excitonically coupled dimer of Zn 132-OH-methylpheophorbide a.

In photosynthesis, pigment–protein complexes achieve outstanding photoinduced charge separation efficiencies through a set of strategies in which excited states delocalization over multiple pigments (“excitons”) and charge-transfer states play key roles. These concepts, and their implementation in bioinspired artificial systems, are attracting increasing attention due to the vast potential that could be tapped by realizing efficient photochemical reactions. In particular, the novo designed proteins provide a diverse structural toolbox that can be used to manipulate the geometric and electronic properties of bound chromophore molecules. However,

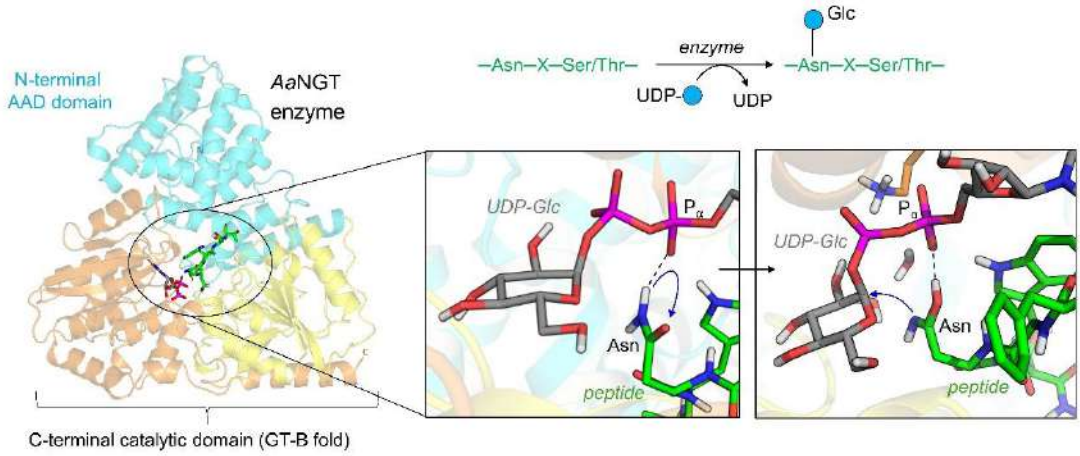
achieving excitonic and charge-transfer states requires closely spaced chromophores, a non-trivial aspect since a strong binding with the protein matrix needs to be maintained. Here, we show how a general-purpose artificial protein can be optimized via molecular dynamics simulations to improve its binding capacity of a chlorophyll derivative, achieving complexes in which chromophores form two closely spaced and strongly interacting dimers. Based on spectroscopy results and computational modelling, we demonstrate each dimer is excitonically coupled, and propose they display signatures of charge-transfer state mixing. This work could open new avenues for the rational design of chromophore–protein complexes with advanced functionalities.

Facile Construction of New Hybrid Conjugation via Boron Cage Extension.
F. Sun, S. Tan, H.-J. Cao, C.-S. Lu, D. Tu, J. Poater, M. Solà, H. Yan.
J. Am. Chem. Soc., 145 (2023) 3577.



We report a new molecular design for conjugation extension, denoted as fusion from a 2D aromatic ring and a 3D boron cluster. By virtue of this boron cage extension strategy, a library of boron cluster-cored tricyclic compounds with varying molecular skeletons can be quickly constructed based on one-pot Pd-catalyzed B–H activation and cascade annulation of nido-carboranes and N-heterocycles with alkynes. These new hybrid tricyclic molecular systems possess an unusual conjugation effect that determines excellent properties such as enhanced thermal stability, generation of new absorption bands, extremely red-shifted emissions (up to 230 nm), and tunable emissions covering from blue to red with Φ up to 61% in the solid state. In sharp contrast, these properties are absent for the corresponding non-fused structures and classical 2D-fused aromatic systems. The present study provides a paradigm to rationally construct boron cluster-cored polycyclic molecules for potential applications.

Molecular basis for bacterial N-glycosylation by a soluble HMW1C-like N-glycosyltransferase.
B. Piniello, J. Macías-León, S. Miyazaki, A. García-García, I. Compañón, M. Ghirardello, V. Taleb, B. Veloz, F. Corzana, A. Miyagawa, C. Rovira*, R. Hurtado-Guerrero*.
Nat. Comms., *14* (2023) 5785.



Proteins are biomolecules essential for life. Most proteins need to be altered after being synthesized, a process named post-translational modifications. One of the most important post-translational modifications is N-glycosylation, in which a sugar molecule becomes attached to an asparagine residue (amino acid) in the protein. Other sugars can subsequently attach to the initial one, forming complex branches that are crucial for the stability of the protein and its correct functioning. Many N-glycosylated proteins, such as the spike protein of SARS-CoV-2, are therapeutic targets.

N-glycosylation is usually initiated by an oligosaccharyltransferase enzyme (OST), that binds a specific oligosaccharide (a short sugar chain) to specific asparagine residues in proteins. It was recently discovered that a bacterial enzyme, identified as soluble N-glycosyltransferase (NGT), could perform a simplified form of N-glycosylation using a single sugar molecule, which could have biotechnological applications (e.g. optimization of the glycan decoration of pharmaceuticals).

In this study the researchers discovered that *Aa*NGT uses a particular pair of basic/acidic residues to recognize the amino acid sequence where the crucial asparagine is located. Furthermore, they used QM/MM MD simulations to uncover the enzyme catalytic mechanism. In this mechanism, the asparagine residue needs to be in its imidic form to react, and the donor substrate itself, rather than an enzyme residue as in other glycosyltransferase enzymes, acts as the general base. These findings are not only significant for enhancing our understanding of NGTs but also open up novel mechanistic pathways for achieving glycosylation that diverges from the most established mechanisms in GTs. Additionally, the knowledge inferred from this work might serve to engineer these enzymes to use them for biotechnological applications such as the synthesis of customed N-glycans in molecules as important as antibodies.

A Step Forward toward Selective Activation/Inhibition of Bak, a Pro-Apoptotic Member of the Bcl-2 Protein Family: Discovery of New Prospective Allosteric Sites Using Molecular Dynamics
Guillem Vila-Julià, Juan J. Perez, and Jaime Rubio-Martinez
J. Chem. Inf. Model. 63(2023) 3544–3556

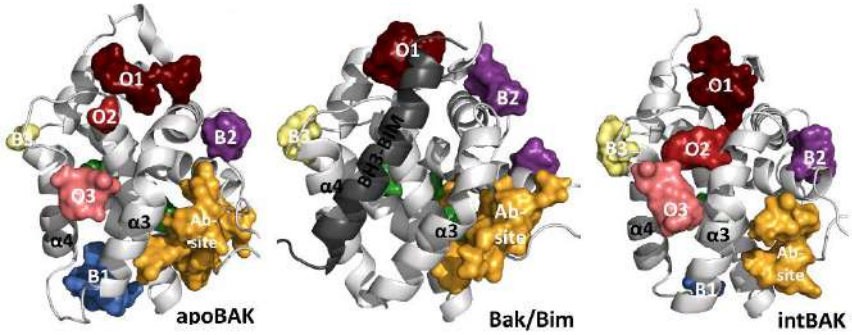


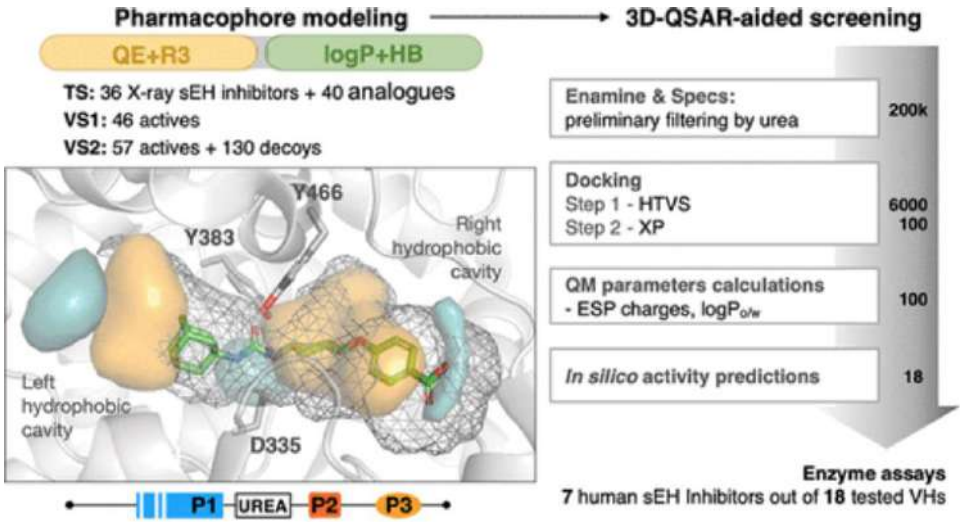
Figure. Bak hotspots identified with FTMap software for representative structures. The orthosteric binding site is represented in three tones of Red, and from the darkest to the lightest correspond to O1-O3 respectively. The Ab-site is represented in Amber, the Rear-site in Green, the B1 in Blue, B2 in Purple and B3 in Pale-Yellow. Hotspots from apoBak complexes, hotspots from intBak complexes and hotspots from Bak/Bim complexes.

Bak, a pro-apoptotic member of the Bcl-2 family, share a common structure with other members of the same family. Bak is similar in structural terms not only with other pro-apoptotic members such as Bax, but also with the anti-apoptotic members, which have an opposite role in apoptosis when comparing to Bak. Members of Bcl-2 family of proteins exhibit and extremely similar orthosteric binding site, region where the endogenous activators bind. This similarity raises a selectivity problem that difficult the identification of new drugs capable of selectively alter Bak activation. An alternative activation site triggered by antibodies has been identified. However, an exhaustive study to identify cryptic pockets as prospective allosteric sites has not yet been performed. Therefore, in this article, we aimed to characterize novel hotspots in Bak structure. To do so, we have used three different Bak systems: Bak on its apo form, Bak in complex with an endogen activator (Bim) and an intermediate form, constructed by removing Bim from the previous complex, allowing to explore all the conformational space between the first two complexes. For all three complexes, we have carried out several MD simulations with two different sampling techniques, conventional MD (cMD), and Gaussian accelerated MD simulations (GaMD). Known binding sites such as the orthosteric binding site and the site triggered by antibodies were detected, as well as novel cryptic pockets, including the Rear-site, B1, B2 and B3. Some of the novel pockets have been described previously in other members of the Bcl-2 family but not for Bak.

Screening and Biological Evaluation of Soluble Epoxide Hydrolase Inhibitors: Assessing the Role of Hydrophobicity in the Pharmacophore-Guided Search of Novel Hits.

J. Vázquez, T. Ginex, A. Herrero, C. Morisseau, B. D. Hammock, F. J. Luque

J. Chem. Inf. Model, *63* (2023) 3209.



The human soluble epoxide hydrolase (sEH) is a bifunctional enzyme that modulates the levels of regulatory epoxy lipids. The hydrolase activity is carried out by a catalytic triad located at the center of a wide L-shaped binding site, which contains two hydrophobic subpockets at both sides. On the basis of these structural features, it can be assumed that desolvation is a major factor in determining the maximal achievable affinity that can be attained for this pocket. Accordingly, hydrophobic descriptors may be better suited to the search of novel hits targeting this enzyme. This study examines the suitability of quantum mechanically derived hydrophobic descriptors in the discovery of novel sEH inhibitors. To this end, three-dimensional quantitative structure–activity relationship (3D-QSAR) pharmacophores were generated by combining electrostatic and steric or alternatively hydrophobic and hydrogen-bond parameters in conjunction with a tailored list of 76 known sEH inhibitors. The pharmacophore models were then validated by using two external sets chosen (i) to rank the potency of four distinct series of compounds and (ii) to discriminate actives from decoys, using in both cases datasets taken from the literature. Finally, a prospective study was performed including a virtual screening of two chemical libraries to identify new potential hits, which were subsequently experimentally tested for their inhibitory activity on human, rat, and mouse sEH. The use of hydrophobic-based descriptors led to the identification of six compounds as inhibitors of the human enzyme with IC50 < 20 nM, including two with IC50 values of 0.4 and 0.7 nM. The results support the use of hydrophobic descriptors as a valuable tool in the search of novel scaffolds that encode a proper hydrophilic/hydrophobic distribution complementary to the target's binding site.

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Identification of novel 1,2,3-triazole isatin derivatives as potent SARS-CoV-2 3CLpro inhibitors via click-chemistry-based rapid screening
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Charge Regulation Triggers Condensation of Short Oligopeptides to Polyelectrolytes
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Controlling the Diradical Character of Thiele Like Compounds
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Strengthened cooperativity of DNA-based cyclic hydrogen-bonded rosettes by subtle functionalization
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Control of Substrate Conformation by Hydrogen Bonding in a Retaining β-Endoglycosidase
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Screening and Biological Evaluation of Soluble Epoxide Hydrolase Inhibitors: Assessing the Role of Hydrophobicity in the Pharmacophore-Guided Search of Novel Hits
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Artificial Neural Network-Derived Unified Six-Dimensional Potential Energy Surface for Tetra Atomic Isomers of the Biogenic [H, C, N, O] System
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On the existence of collective interactions reinforcing the metal-ligand bond in organometallic compounds
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The nature of the electronic ground state of M2C (M = Ti, V, Cr, Zr, Nb, Mo, Hf, Ta, and W) MXenes
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Glycosidase mechanisms: Sugar conformations and reactivity in endo- and exo-acting enzymes
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A hotspot for posttranslational modifications on the androgen receptor dimer interface drives pathology and anti-androgen resistance
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Bis(Vinylenedithio)-Tetrathiafulvalene-Based Coordination Networks
(2023) Chemistry - A European Journal, 29 (8), art. no. e202203138

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Trans-cyclosulfamidate mannose-configured cyclitol allows isoform-dependent inhibition of GH47 α-d-mannosidases through a bump-hole strategy
(2023) Chemical Science, 14 (46), pp. 13581 - 13586

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Unraveling the role of thermal fluctuations on the exciton structure of the cryptophyte PC612 and PC645 photosynthetic antenna complexes
(2023) Frontiers in Molecular Biosciences, 10, art. no. 1268278

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Unlocking the predictive power of quantum-inspired representations for intermolecular properties in machine learning
(2023) Digital Discovery, 3 (1), pp. 99 - 112

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Crystal properties without crystallinity? Influence of surface hydroxylation on the structure and properties of small TiO2 nanoparticles
(2023) Nanoscale, 15 (10), pp. 4809 - 4820

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Systematic Characterization of Electronic Metal-Support Interactions in Ceria-Supported Pt Particles
(2023) Journal of Physical Chemistry C, 127 (36), pp. 17700 - 17710

93. García-Romeral N., Morales-García I., Viñes F., Moreira I.D.P.R., Illas F.
How does thickness affect magnetic coupling in Ti-based MXenes
(2023) Physical Chemistry Chemical Physics, 25 (26), pp. 17116 - 17127

94. Jimenez-Orozco C., Flórez E., Viñes F., Rodriguez J.A., Illas F.
Ethylene Hydrogenation Molecular Mechanism on MoCy Nanoparticles
(2023) Journal of Physical Chemistry C, 127 (16), pp. 7666 – 7673

95. Optimal Pt-Au alloying for efficient and stable oxygen reduction reaction catalyst
X. Xie, V. Briega-Martos, R. Farris, M. Dopita, M. Vorokhta, T. Skála, I. Matolínová, K.M. Neyman, S. Cherevko, I. Khalakhan.
(2023) ACS Appl. Mater. Interfaces 15, 1192-1200

96. Effects of oxygen adsorption on optical properties of Ag nanoparticles
E. Zerbato, R. Farris, G. Fronzoni, K.M. Neyman, M. Stener, A. Bruix
(2023) J. Phys. Chem. A 127, 10412-10424.

Other Activities

PHD THESES 2023

Computational modelling of the pH effect on intrinsically disordered proteins
Cristian Privat Contreras
Facultat de Química, Universitat de Barcelona
Jaime Rubio, Sergio Madurga
March 2023

Tuning the Composition and Dimensionality of Transition Metal Carbides as Possible Catalysts for Green Chemistry Related Reactions.
Martí López Berbel
Facultat de Química, Universitat de Barcelona.
PhD program: Theoretical Chemistry and Computational Modelling.
Supervisors: F. Viñes, F. Illas.
March 2023

MXene Materials for CO_2 Capture and Transformation.
Anabel Jurado Mañas
Facultat de Química, Universitat de Barcelona.
PhD program: Theoretical Chemistry and Computational Modelling.
Supervisors: Á. Morales-García, F. Illas.
June 2023

Conception assistée par ordinateur des modulateurs de polymérisation de la tubuline
Maxim Shevelev
Universite of Barcelona and Universite of Strasbourg
Chimie / Chémoinformatique
Jaime Rubio Martínez; Alexandrre VARNEK; Dragos HORVATH and Marta Cascante Serratosa
September 2023

Computational insights into carbohydrate epimerase mechanisms
Oriol Esquivias Bautista de Lisbona
Facultat de Química, Universitat de Barcelona.
Doctoral programme in Organic Chemistry
Carme Rovira
November 2023

Computational modelling to study mèdium effect over molècules and biopolymers of interest in biomedicine
Haruna Luz Barazorda Ccahuana
Facultat de Química, Universitat de Barcelona
Francesc Mas
Novembre 2023

Rational-Design of new candidates targeting Bak and Bombesin receptors in Cancer
Guillem Vila i Julià
Escuela Técnica Superior de Ingeniería Industrial. UPC
Bioinformática
Jaime Rubio Martínez and Juan Jesús Pérez González
November 2023

Multiscale Modelling of CO_2 Hydrogenation Reactions on Ni-Based Catalysts.
Pablo Lozano Reis
Facultat de Química, Universitat de Barcelona.
PhD program: Theoretical Chemistry and Computational Modelling.
Supervisors: R. Sayós, F. Illas.
November 2023

Developing non-equilibrium approaches to control the self-assembly of funcional supramolecular sysyems.
James Daniel Nicholas
ETH Zurich
PhD Programme MaP Doctoral School
Supervisor/s: Prof. Dr. Andrew J deMello, Prof. Dr. Josep Puigmartí Luis, Prof. Dr. Salvador Pané Vidal
Desembre 2023

Prediction of partition coefficients for systems of micelles using DFT
Leila Saranjam
Facultat de Química, Universitat de Barcelona
Sergio Madurga
2023

Master Theses 2023

CFD Validation of Atmospheric Gas Dispersion: A comparison with Gaussian Models and Experimental Data.
Carlos Troyano Ferrer
Facultat de Química, Universitat de Barcelona.
Master of Chemical Engineering
Alexandra Plesu Popescu / Ruben Cabello Gallego
February 2023.

Contribution to the study of the rigid polyester production process.
Fátima Zhora Benali Ouhazem
Facultat de Química, Universitat de Barcelona.
Master of Chemical Engineering
Jordi Bonet i Ruiz / Ruben Cabello Gallego
February 2023.

Contribution to the study of the units of a sylvinite ore processing plant.
Juan Francisco Otero Belcastro
Facultat de Química, Universitat de Barcelona.
Master of Chemical Engineering
Jordi Bonet i Ruiz / Ruben Cabello Gallego
February 2023.

Computational Calculation of the Fluorescence Spectrum of a COX-2-specific Fluorogenic Probe Inside the Human COX-2
Álex Pérez Sánchez
Facultat de Farmàcia i Ciències de l'Alimentació, Universitat de Barcelona.
Master in Theoretical Chemistry and Computational Modelling
Carles Curutchet (UB), Àngels González-Lafont (UAB) & José M. Lluch (UAB)
June 2023.

Study of organic diradicals derived from indolo[3,2-b] carbazole and extension to the design of organic π-tetraradicals: influence of geometry, conjugation, aromaticity and multiplicity.
Sergi Betkhoshvili
Facultat de Química, Universitat de Barcelona.
Master on Theoretical Chemistry and Computational Modelling
Josep Maria Bofill Villà, Jordi Poater Teixidor.
June 2023.

Life Cycle Analysis in the Production of PHA Biopolymers
Ruben Dario Plata Manjarrez
Facultat de Química, Universitat de Barcelona.
Master of Environmental Engineering
Alexandra Plesu Popescu / Yen Keong Cheah
June 2023.

Synthesis of novel building blocks for the formation of dissipative porous supramolecular polymer networks
Júlia Soler Vilà
Facultat de Química, Universitat de Barcelona.
Master in Organic Chemistry
A. Sorrenti
June 2023.

Contribution to the study of Regenerative Thermal Oxidator (RTO) units
Biel Martí Ferre
Facultat de Química, Universitat de Barcelona.
Master of Chemical Engineering
Alexandra Plesu Popescu / Jordi Bonet i Ruiz
July 2023.

Development and application of a ReaxFF force field for the hydrogenation of CO_2 on ruthenium functionalized zeolites
Christian Dominguez Dalmases
Facultat de Química, Universitat de Barcelona.
Master Erasmus Mundus on Theoretical Chemistry and Computational Modelling
Ramón Sayós Ortega
July 2023.

Insights into the Catalytic Mechanism of Maltodextrin Phosphorylase using QM/MM MD: Assessment of a Long-Lived Oxocarbenium Ion Intermediate
David J. E. Delima
Facultat de Química, Universitat de Barcelona.
Theoretical Chemistry and Computational Modelling (TCCM)
Carme Rovira
July 2023

Charge Separation versus Charge Transport in 2D Covalent Organic Frameworks for Optoelectronic applications.
Arnau Garcia Duran
Facultat de Química, Universitat de Barcelona.
Master in Atomistic and Multiscale Computational Modelling in Physics, Chemistry and Biochemistry
Supervisor: Maria Fumanal
July 2023.

Graphyne-inspired new topologies for triphenylmethyl radical-based 2D Covalent Organic Frameworks
Daniel Blas Buch
Facultat de Química, Universitat de Barcelona.
Master in Theoretical Chemistry and Computational Modelling
Supervisors: Jordi Ribas and Stefan T. Bromley
July 2023.

Control of π-conjugation in organic systems through electric-field-induced isomerizations
Arnau Cortés Llamas
Facultat de Química, Universitat de Barcelona.
Master in Atomistic and Multiscale Computational Modelling in Physics, Chemistry and Biochemistry
Supervisor: Jordi Ribas and Stefan T. Bromley
July 2023.

Synthesis of Zinc-porphyrin dyads for use in liposomal photoinduced trans-membrane electron transport
Ingrid Delgado Aguilera
Facultat de Química, Universitat de Barcelona.
Organic Chemistry Master
Dr. Bart Limburg
July 2023.

Towards the understanding of the Structure-Action Relationship of CutC as a relevant target for the treatment of Cardiovascular Diseases
Mireia Gómez-Gordo
Master in Biomedicine - UB
Supervisor/s: C. Estarellas
July 2023.

Unveiling the full 3D structure of α2β2γ1 AMPK complex: towards the understanding of allosteric mechanism
Joel M. Bascuas
Master in Biotechnology - UB
Supervisor/s: C. Estarellas
July 2023.

Development of ab initio-based Force Field for the MIL53Cr Metal-Organic Framework.
Sergi Lou Alonso
Facultat de Química, Universitat de Barcelona.
Química de Materials Aplicada
Supervisor/s. J. Cirera
Juliol 2023.

Estudi Computacional de la Reacció de Sonogashira entre Alquins Terminals i Iodobenzens: Efectes del Substrat i del Lligand.
Sonia Milán Muñoz
Facultat de Química, Universitat de Barcelona.
Química de Materials Aplicada
Supervisor/s. J. Jover
Juliol 2023.

Investigation of the Water Splitting Reaction on ZnO Surfaces in the Excited State.
Miquel Allès Coll
Facultat de Química, Universitat de Barcelona.
Erasmus Mundus Theoretical Chemistry and Computational Modelling
Supervisors: Á. Morales-García, F. Viñes.
July 2023.

Tuning MXenes towards their Use in Photocatalytic Water Splitting.
Diego Ontiveros Cruz
Facultat de Química, Universitat de Barcelona.
Atomistic and Multiscale Computational Modelling in Physics, Chemistry and Biochemistry
Supervisors: F. Viñes, C. Sousa.
July 2023.

Determining the conformational plasticity of Choline trimethylamine-lyase from Klebsiella pneumoniae
Fajar Puteras
Erasmus Mundus Master in Chemical Innovation and Regulation – UB, UAlg, UniBo
Supervisor/s: C. Estarellas
September 2023.

ORGANIZATION OF CONGRESSES 2023

International Symposium "Density Functional Theory, Sorption and Catalysis"
Garching b. Munich (Germany)
Congress organization
Chairman and Organizers: .Konstantin Neyman (UB), Sven Krüger (TU München)

Symposium "Chemical Reactivity: Computational Methods and Applications"
Zaragoza (Spain)
XXXIX Biennial meeting of the Spanish Royal Chemical Society
Chairman or Organizers: M. Swart and C. Rovira

Reunió de Química Teòrica i Computacional de la Societat Catalana de Química
Barcelona (Spain), January 2023
M. Deumal (she was one of the chairs of the conference)

EuChemS CompChem 2023 - European Conference on Computaqonal & Theoretical Chemistry
Thessaloniki (Greece), August 2023
M. Deumal (participation in the scientific committee)

Walter Thiel's Award of EuChemS-DCTC. **2023 Edition**.
M. Deumal (participation in the scientific committee)

Workshop sobre Metodologies creatives en gastronomía
Membre del comité organitzador.F. J. Luque
17/04/2023 Edifici Històric de la Universitat de Barcelona

Science & Cooking World Congress Barcelona 2023
Vicepresident del comitè organitzador, F. J. Luque
11-13 de novembre de 2023

International Conference On Nanomedicine And Nanobiotechnology – ICONAN 2024
Park Scientific of Barcelona, Barcelona, Spain
Mohit Kumar

Scientific conferences and Meetings 2023

1ª Reunió de Química Teòrica i Computacional
Institut d'Estudis Catalans, Barcelona (Spain)
30/01/2023-31/01/2023

Environment effects change FRET distributions in a fluorophore-tagged disordered protein (talk)
D. Gonzalo, J. Juárez-Jiménez, C. Curutchet
Using molecular dynamics simulations with organic solvent/water mixtures to identify imidazoline I2 receptor binding sites (poster)
B. Ozaydin, C. Griñán-Ferré, A. Bagán, M. Pallàs, C. Escolano, C. Curutchet, J. Juarez-Jiménez
Extending the MST model to large biomolecular systems: parametrization of the ddCOSMO-MST continuum solvation model (poster)
R.D. Cunha, S. Romero, F. Lipparini, F.J. Luque, C. Curutchet
Characterizing drug binding through Förster Resonance Energy Transfer (poster)
O. Ergun, M. Castell, X. Barril, C. Galdeano, C. Curutchet
3D and 2D aromaticies: Like oil and water? The case of benzocarborane derivatives and 3D/3D fusion (poster)
J. Poater
Conversió del CO_2 en combustibles lleugers utilitzant catàlisi single-atom de Ru suportat en silicalita (comunicació oral)
M. Cánovas, A. Gracia, G. Alonso, R. Sayós, P. Gamallo
Es pot descriure la variació de pKa d'un polipèptid en funció del pH mitjançant isotermes de complexació? (poster)
Privat, C.; Madurga, S.; Rubio-Martinez, J.; Mas, F
Caracterització de les isotermes de protonació de polielectròlits que mimetitzen la matèria orgànica dissolta
Orradre, J.; Naranjo, D.; Blanco, P.M.; David, C.; Rey-Castro, C.; Madurga, S.; Garcés, J.L.; Mas, F.
Obrint els ulls en l'al·losterisme de la proteïna proapoptòtica Bak
Vila-Julià, G.; J. Perez, J.; Rubio-Martinez, J
Computer-aided drug design of hemagglutinin fusion peptide inhibidors (poster)
Barmpidi, K.; Luque, F.J.; Estarellas, C.
Activator vs inhibitor of β-ampk: towards the understanding of isoform selectivity (poster)
Barmpidi, K.; Luque, F.J.; Estarellas, C.
Factors moleculars que regulen els biometabòlits de la microbiota intestinal: El cas específic de Choline Trimethylamine-Lyase (poster)
Gómez, M.; Estarellas, C.
Millora dels Temps de Relaxació d'Imants Unimoleculars (pòster)
A. Silvestre-Llora, D. González, S. Gómez-Coca, E. Ruiz
A Theoretical Analysis Of Magnetic Coupling In MXene Ti_2C (Poster)
N. García-Romeral

MasterQuímica XVIII
Universitat de Barcelona
23/05/2023

Efecte dels additius en la contaminació de nanoplàstics i metalls pesats en efluents andins (poster)
Paco-Chipana, M.; Centeno-Lopez, A.E.; Barazorda-Ccahuana, H.L.; Mas, F.; Madurga, S.
Simulació de nanogels termosensibles a la mesoescala (poster)
Valero, D.; Blanco, P.M.; Mas, F.; Madurga, S.
MXens com a Fotocatalitzadors del Trencament de l'Aigua (Poster)
D. Ontiveros

10th International Conference on Sustainable Solid Waste Management
21/06/2023

Modelling of the performance of hydrophobic and hydrophilic/hydrophobic membranes for nitrogen recovery from wastewaters (poster)
Serra-Toro, A.; da Silva, C.; Madurga, S.; Astals, S.; Dosta, J.; Mas, F.

17th International Congress of Quantum Chemistry
Comenius University, Bratislava (Slovakia)
26/06/2023-01/07/2023

Environment effects change FRET distributions in a fluorophore-tagged disordered protein (poster)
D. Gonzalo, J. Juárez-Jiménez, C. Curutchet
Multiscale investigation of the structural basis for photoacclimation in the cryptophyte alga PC577 and PE545 antenna complexes (poster)
R.D. Cunha, C. Curutchet
Förster Resonance Energy Transfer Applied to Drug Design (poster)
O. Ergun, M. Castell, X. Barril, C. Galdeano, C. Curutchet
On the impact of thermal fluctuations on the exciton structure of the PC612 and PC645 antenna complexes: A dual classical/quantum molecular dynamics study (poster)
B. Ozaydin, C. Curutchet

1ª Jornada de Recerca i Divulgació de Doctorat de la UB
Universitat de Barcelona, Barcelona (Spain)
19/05/2023

Environment effects change FRET distributions in a fluorophore-tagged disordered protein (poster)
D. Gonzalo, J. Juárez-Jiménez, C. Curutchet
Using molecular dynamics simulations with organic solvent/water mixtures to identify imidazoline I2 receptor binding sites (poster)
B. Ozaydin, C. Griñán-Ferré, A. Bagán, M. Pallàs, C. Escolano, C. Curutchet, J. Juarez-Jiménez
Characterizing drug binding through Förster Resonance Energy Transfer (poster)
O. Ergun, M. Castell, X. Barril, C. Galdeano, C. Curutchet
Extending the MST model to large biomolecular systems: parametrization of the ddCOSMO-MST continuum solvation model (poster)
R.D. Cunha, S. Romero, F. Lipparini, F.J. Luque, C. Curutchet

XIV Jornada de Recerca de la Facultat de Farmàcia i Ciències de l'Alimentació
Universitat de Barcelona, Barcelona (Spain)
30/11/2023

Environment effects change FRET distributions in a fluorophore-tagged disordered protein (poster)
D. Gonzalo, J. Juárez-Jiménez, C. Curutchet
Extending the MST model to large biomolecular systems: parametrization of the ddCOSMO-MST continuum solvation model (poster)
R.D. Cunha, S. Romero, F. Lipparini, F.J. Luque, C. Curutchet

IQTC/QTMC Meeting 2023 of the Institute of Theoretical and Computational Chemistry
Universitat de Barcelona, Barcelona (Spain)
18/09/2023-19/09/2023

Using molecular dynamics simulations with organic solvent/water mixtures to identify imidazoline I2 receptor binding sites (poster)
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Multiscale investigation of the structural basis for photoacclimation in the cryptophyte alga PC577 and PE545 antenna complexes (poster)
R.D. Cunha, C. Curutchet
Time optimal control of molecular spin qudits (poster)
M. Alsina, J. M. Bofill, G. Albareda, I. de P. R. Moreira
Unveiling non-classical mechanism of glycoside hydrolases (talk)
I. Cuxart
Flexible weak polyelectrolytes as effective rigid objects limitations of the Site Binding model (poster)
Orradre, J.; Blanco, P.M.; Madurga, S.; Mas, F.; Garcñes, J.L.
Role of conformational plasticity in selective direct activation mechanism of AMPK isoforms"
Estarellas, C.
Towards a unified understanding of allosteric AMPK activators via funnel-shaped restraint metadynamics (poster)
Evans, R.; Luque, F.J.; Estarellas, C.
On the sterol selectivity of the N-terminal domain of NPC1L1 (poster)
Valdivia, A.; Luque, F. J.; Llabrés, S.
Towards a new strategy for fighting Mycobacterium tuberculosis through the reductase-trHbN complex (poster)
Barmpidi, K.; Estarellas, C.; Luque, F. J.
Systematic Study of the Dissociation of CO Molecule on Transition Metal Surfaces (Poster)
D. Vázquez-Parga
MXenes as Photocatalytic Materials for Water Splitting (Poster)
D. Ontiveros
Single-Atom Catalysts based on PtN_x for the Electrocatalytic Chlorine Evolution Reaction: A Theoretical Study (Poster)
L. Meng
The Thickness Influence On Magnetic Coupling On Ti-Based MXenes (Poster)
N. García-Romeral
Computational Pourbaix Diagrams for MXenes: A Key Ingredient Toward Proper Theoretical Electrocatalytic Studies (Poster)
M. López
Identifying the Atomic Layer Stacking of Mo_2C by Probe Molecule Adsorption (Poster)
A. Jurado

Digitally Driven Biotechnology Symposium
Danish Technical University, Copenhagen (Denmark)
26/10/2023

Fundamental aspects of enzyme catalysis to inform biotechnology approaches (Keynote)
C. Rovira

Trends in Enzyme Catalysis. Merging Theory and Experiments. TrEnCa 2023
Benicàssim (Spain)
30-1/11-12/2023

QM/MM studies of protein glycosylation reactions (invited speaker)
C. Rovira

European Conference on Computational & Theoretical Chemistry "Exploring Molecular Space" (EuChemS CompChem 2023)
Olympic Museum, Thessaloniki (Greece)
27/08/2023-31/08/2023

Investigating the allosteric inhibition mechanism of I2 ligands in MAO-B using MD simulations with organic solvent/water mixtures (poster)
B. Ozaydin, C. Griñán-Ferré, A. Bagán, M. Pallàs, C. Escolano, C. Curutchet, J. Juarez-Jiménez
Förster Resonance Energy Transfer Applied to Drug Design (poster)
O. Ergun, M. Castell, X. Barril, C. Galdeano, C. Curutchet
Multiscale investigation of the structural basis for photoacclimation in the cryptophyte alga PC577 and PE545 antenna complexes (poster)
R.D. Cunha, C. Curutchet

XXII Simpósio Brasileiro de Química Teórica (SBQT)
Universidade Federal Fluminense, Niterói (Brazil)
23/10/2023-26/10/2023

Multiscale investigation of the structural basis for photoacclimation in the cryptophyte alga PC577 and PE545 antenna complexes (talk)
R.D. Cunha, C. Curutchet

II Simposio de Jóvenes Investigadores, Real Academia Nacional de Medicina.
Madrid, Spain
17/052023.

Lectura y eliminación del análogo de fosfonio de la trimetillisina por proteínas epigenéticas (invited talk)
J. Poater

XXXIX Reunión Bienal de la Real Sociedad Española de Química.
Zaragoza (Spain)
25/06/2023

Aromaticity and Extrusion of Benzenoids Linked to [o-COSAN]−: Clar has the answer (talk)
J. Poater
Enzymatic hydrolysis of human milk oligosaccharides. The molecular mechanism of Bifidobacterium bifidum lacto-N-biosidase (flash talk, poster)
I. Cuxart, J. Coines, O. Esquivias, M. Faijes, A. Planas,X. Biarnés, C. Rovira
Enzymatic C4 Epimerization of UDP-Glucuronic Acid: Precisely Steered Rotation of a Transient 4-Keto Intermediate for Inverting Reaction without Decarboxylation (Flash talk and poster)
O. Esquivias, A.J.E. Borg, J. Coines, B. Nideztky, C. Rovira
Uncovering catalytic mechanisms of inverting glycosyltransferases involved in protein glycosylation: β-1,6-N-acetylglucosaminyltransferase V (MGAT5) and protein O-fucosyltransferase 1 (POFUT1) (Oral presentation)
B. Piniello, L. Wu, G.J. Davies, R.S. Haltiwanger, R.Hurtado-Guerrero, C. Rovira
Ionic 2D Materials (comunicación oral)
E. Ruiz
Improvement of the Magnetic Properties of Single Molecule Magnets by Encapsulation in Organic Hosts (comunicación oral)
S. Gómez-Coca, A. Silvestre-Llora, M. Amoza, D. González, E. Ruiz
Base Metal-catalyzed Sonogashira Cross-coupling: New Directions from Non-classical Reaction Mechanisms (comunicación oral)
J. Jover, O. Loveday
The Importance of Dihydrogen Interactions for the Molecular Configuration of Triglycerides (comunicación oral)
G. Aullón, J. Echeverría, L. Bayés-García, T. Calvet, M. A. Cuevas-Diarte, S. Alvarez
Computational Chemistry: Beyond the Numbers (Plenary session)
F. Illas
How Does Thickness Affect Magnetic Coupling on Ti Based MXenes (Poster)
N. García-Romeral

Charge Reservoirs in an Expanded Halide Perovskite Analog: Enhancing High-Pressure Conductivity through Redox-Active Molecules.
Matheu, R.; Umeyana, D.; Karunadasa, H.

21st European Carbohydrate Symposium
Maison de la Chimie, Paris (France)
11/07/2023

The catalytic reaction mechanism of the β-galactocerebrosidase enzyme deficient in Krabbe disease (oral presentation)
A. Nin-Hill, C. Rovira
How glycosidases operate: combining crystallography and quantum mechanics to uncover new mechanisms (Duo oral communication)
C. Rovira, M. Morais
Structural and mechanistic insights into the cleavage of clustered O-glycan peptides by mucinases (Oral presentation)
Q. Liao
Conformational Space of Glucose Mono- and Di-saccharides: Comparison of GLYCAM06j and CHARMM36 Force Fields (Poster)
Q. Liao
Uncovering catalytic mechanisms of inverting glycosyltransferases involved in protein glycosylation: β-1,6-N-acetylglucosaminyltransferase V (MGAT5) and protein O-fucosyltransferase 1 (POFUT1) (Oral presentation)
B. Piniello, L. Wu, G.J. Davies, R.S. Haltiwanger, R.Hurtado-Guerrero, C. Rovira

32nd Annual Computational Neuroscience Meeting
Congress Center Leipzig, Leipzig (Germany)
18/07/2023

The impact of photopharmacology on brain circuits research: present and future prospects (invited speaker)
A. Nin-Hill, M. Alfonso-Prieto

Gordon Research Conference (GRC) on Carbohydrate-Active Enzymes for Glycan Conversions
Proctor Academy, Andover (USA)
23-28/07/2023

Simulation of glycosyltransferase catalytic mechanisms (invited speaker)
C. Rovira

IUPAC – CHAINS 2023.

The Hague (The Netherlands)
20/08/2023

Construction of Hybrid Conjugation via Boron Cage Extension (talk)
J. Poater

ICIQ School
Tarragona (Spain)
13/09/2023

Z. Noori

19th European Symposium on Organic Reactivity (ESOR2023).
Amsterdam (The Netherlands)
19/09/2023

Through-Space Stabilization of an Imidazolium Cation by Aromatic Rings (talk)
J. Poater

International Symposium on Chemical Concepts from Theory and Computationa 3 (CCTC2023)
Lyon (France)
11/12/2023

Adjusting UV-Vis Spectrum of Alizarin by Insertion of Auxochromes (poster)
Z. Noori, J. Poater

International workshop on Fundamental Principles of Catalysis
Skoltech, Moscow (Russia)
27-28/11/2023

Effects of oxide supports on transition-metal particles in catalytic nanomaterials (invited lecture, on-line)
K.M. Neyman

Webinar of the MDPI journal "Metals"
On-line
25/05/2023

DFT calculations of the chemical ordering in bimetallic nanocrystallites using a TOP method (invited lecture)
K.M. Neyman

Seminar of the CLINT-Collaborative Research Center CRC 1452 'Catalysis at Liquid Interfaces'
Friedrich-Alexander Universität Erlangen-Nürnberg, Erlangen (Germany)
20/04/2023

Quantifying metal/metal-oxide interface effects in catalysts by combining DFT modelling with experiments (invited lecture)
K.M. Neyman

Seminar of the TUM School of Natural Sciences
Technische Universität München, Garching (Germany)
18/04/2023

Quantifying metal/metal-oxide interface effects in catalysts by combining DFT modelling with experiments (invited lecture)
K.M. Neyman

International Conference "Designing the Future: Electro-, Photo- and Thermochemical Water Splitting" of the COST Action 18234
Brussels (Belgium)
20-22/02/2023

Surprising oxidation of platinum in sub-nano states: Insights from catalytic experiments and DFT modelling (invited lecture)
J.E. Quinlivan, A. Bruix, K.M. Neyman

Modeling and Understanding Hydroxylation of TiO_2 Nanoparticles: One More Step Towards Approaching Realistic Systems (Invited speaker)
F. Illas

Crystal properties without crystallinity? Influence of Surface Hydroxylation on the Structure and Properties of Small TiO_2 Nanoparticles (Poster)
M. Recio-Poo

International Conference "Development of Nanostructured Materials through Computational Modelling" of the COST Action 18234
Haifa (Israel)
17-19/07/2023

Effects of oxide supports on metal particles in catalytic nanomaterials (talk)
K.M. Neyman

IUVSTA-ZCAM Workshop "Metal-Oxide Ultrathin Films and Nanostructures: Experiment Meets Theory"
Zaragoza (Spain)
03-07/07/2023

Oxidation of platinum at sub-nano scale: Insights from catalytic experiments and DFT modelling (talk)
K.M. Neyman, J. Quinlivan, A. Bruix

International Meeting on Nanoalloys (IMN 2023)
Orleans (France)
09-11/05/2023

Nanoalloys of Pt and Pd with Au, Ag and Cu: DFT calculations combined with Topological approach (talk)
K.M. Neyman

Flatlands. Beyond graphene 2023.
Prague (Czech republlic)
25-29 Setember, 2023

Inducing low-lying correlated gapped states in graphene-like 2D-COFs by mechanical strain and stress (talk)
I. de P. R. Moreira
Emergent spin frustration in 2D covalent organic radical frameworks: a potential quantum materials platform (talk)
J. Ribas-Ariño

26th conference on Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction (PRES23)
Thessaloniki (Greece)
Celebration date (8-11/10/2023)

Zeolites for Direct Carbon Dioxide Capture, (talk)
C. Troyano Ferré, R. Cabello, A.E. Plesu Popescu, J. Bonet-Ruiz, P. Gamallo Belmonte, J. Camps
Computational Fluid Dynamics Simulation of a Dead-End Forward Osmosis Cell to Evaluate the Effect of Hydrodynamics on the Permeation Process, (poster)
S. Shahgodari, R. Cabello, J. Labanda, J. Llorens

MIAPbP Workshop: ENGINEERING LIFE: FROM SYSTEM CHEMISTRY, BIOPHYSICS, AND THEORETICAL PHYSICS.
Munich (Germany)
13-24 /March/ 2023

Chirality transfer from a 3D macro shape to the molecular level by controlling asymmetric secondary flows. (Invited oral)
A. Sorrenti

CHIRALITY 2023 33rd International Symposium on Chirality.
Rome (Italy)
24-27/July/2023

Exploiting asymmetric secondary flows to transfer chirality from a 3D macro shape to the molecular level. (Keynote Lecture Invited)
A. Sorrenti

1era REUNIÓ DE QUÍMICA INORGÀNICA I ORGANOMETÀL·LICA de la SCQ

Barcelona, Spain
2nd -3rd February 2023

Microfluidic technologies as an advanced tool for chemistry and materials synthesis
J. Puigmartí-Luis

1st Iberian Symposium on Functional Organic Polymers
Aveiro, Portugal
11-12 May 2023
Functional materials by design via microfluidic technologies
J. Puigmartí-Luis (invited by Prof. M. Souto)
Intramolecular Singlet Fission in Donor-Acceptor Copolymers (talk)
M. Fumanal

18th IEEE International Conference on Nano/Micro Engineered and Molecular Systems (IEEE NEMS 2023)
Jeju, Korea
(14-17 May 2023)
MOFBOTS: Metal-Organic Framework-Based Biomedical Microrobots
J. Puigmartí-Luis (invited by Prof. Hongsoo Choi)

IEEE International Conference on Manipulation, Manufacturing and Measurement on the Nanoscale (IEEE 3M-NANO)
Chengdu, China
(31 July-4 August 2023)
Controlled Materials Engineering via Microfluidic Technologies
J. Puigmartí-Luis (invited by Prof. Zuobin Wang)

International Conference on Manipulation, Automation and Robotics at Small Scales (MARSS)
Abu Dhabi, UAE
10-12 October 2023
Porous crystalline materials in motion
J. Puigmartí-Luis (invited by Prof. Abdon Pena-Francesch and Prof. Hamed Shahsavan)

16th IEEE International Conference on Nano/Molecular Medicine & Engineering (IEEE-NANOMED 2023)
Okinawa, Japan
5-8 December 2023
Controlled Materials Engineering via Microfluidic Technologies
J. Puigmartí-Luis (invited by Prof. Kin Fong Lei)

9th International Conference on Bio-Inspiration in Nice - France
Nice, France
12-14 December 2023
Controlled Materials Engineering via Microfluidic Technologies
J. Puigmartí-Luis (invited by Prof. Frédéric Guittard)

Hamilton Institute Student Seminar Series
Eolas Building, Maynooth University, Maynooth (Ireland)
29/03/2023
Simulation of enzyme reactions in glycoside hydrolases, (talk)
I. Cuxart

XIII Spanish Carbohydrate Meeting
Institut Químic de Sarrià, Barcelona (Spain)
27-29/03/2023
Uncovering catalytic mechanisms of inverting glycosyltransferases involved in protein glycosylation: β-1,6-N-acetylglucosaminyltransferase V (MGAT5) and protein O-fucosyltransferase 1 (POFUT1) (Poster)
B. Piniello, L. Wu, G.J. Davies, R.S. Haltiwanger, R.Hurtado-Guerrero, C. Rovira

GGMM Young Modellers Conference
Hotel Mercure Toulouse Centre Compans, Toulouse (France)
15/05/2023

Investigating desaturation/hydroxylation specificity of the CpFAH12 bifunctional enzyme using multi-scale modelling (poster)
A. Nin-Hill., J. Esque, S. Bengaouera, J. Le Reun, C. Rovira, F. Bordes, I. André

ZCAM and CECAM. Present and future
Zaragoza, Spain
8-9/06/2023

How enzymes work. Insight from computer simulation (invited speaker)
C. Rovira

13th International Symposium on Polyelectrolytes
Praga, Republica Txeca
28/08/2023

Adsorption of flexible proteins in the "wrong side" of the isoelectric point: Casein macropeptide as a model System
Blanco, P.M.; Acheonti, M.M.; Garcés, J.L.; Madurga, S.; Mas, F.; Baieli, M.F.; Narambuena, C.F.
Coupling of ionization and conformational degrees of freedom in polyprotic molecules and polyelectrolytes (poster)
Orradre, J.; Mas, F.; Madurga, S.; Blanco, P.; Garcés, J.L.

45º Congreso de la SEBBM.
Zaragoza, Spain
05/09/2023

Identification of distinctive immune-metabolic phenotypes in colorectal cancer with potentialimplications in the design of combined therapies (poster)
Cascante, M.; Pedrosa, L.; Foguet, C.; Cuatrecasas, M.; Camps, J.; Lopez-Blanco, D.; Gorría, T.; Oliveres, H.; Rojas, M.; de Atauri, P.; Mas, F.; Tarrado-Castellarnau, M.; Marín, S.; Madurga, S.; Maurel, J.

6th International Conference: Wastes - Solutions, Treatments and Opportunities.
Coimbra, Portugal
06/09/2023-08/09/2023

Ammoniacal Nitrogen recovery from swine slurry using a gas-permeabble membrane: Effect of pH and feedto-trapping volume ratio
Serra-Toro, A.; Astals, S.; Valentino, F.; Mas, F.; Dosta, J.

EMBO Workshop. Computational models of life: From molecular biology to digital twins.
Girona, Spain
26/11/2023

Metabolic Modelling of pro-Inflammatory Human Macrophages. The Role of the SARS-CoV2 Cytokine Storm (poster)
Madurga, S.; Sánchez-García, S.; Povo-Retana, A.; Fariñas, M.; Landauro-Vera, R.; Prieto, P.; Foguet, C.; Marin, S.; Aleixandre, N.; Boscá, L.; Cascante, M.

Targeting RAS. New challenges and avenues
Salamanca (España)
13/September/2023

A new small molecule binds directly to oncogenic KRAS increasing dowmstream KRAS signalling while reducing colorectal cancer cells (CRC) viability.
Abuasaker, B.; Brun, S.; Engel R. M.; Boka, H.; McMurrick P.J.; Jaumot, M.; Pujol, M.D.; Rubio-Martínez, J.; Abud, H.; Agell, N.

Modeling interactions in biomolecules IX
Průhonice (Czech Republic)
10/September/2023

Fragment dissolved molecular dynamics, uncovering newopportunities in drug design.
Peralta-Moreno, MN.; Granadino-Roldán, JM.; Rubio-Martinez, J.
Quest for compounds that selectively activate the pro-apoptotic Bax protein.
de-Moya, N.; García-Jareño, A.; Orzáez, M.; Rubio-Martinez, J.
Establishing a binding model for bombesin to bombesinreceptors
Vila-Julià G.; Rubio-Martinez, J.; Pérez, JJ.
Markov state models with Fragment Dissolved Molecular Dynamics as a step forward in drug design
Peralta-Moreno, MN.; Rodríguez-García, A.; Granadino-Roldán, JM.; Rubio-Martinez, J.
HYPHAR: A Journey from Continuum Solvation Models to Virtual Screening in Drug Discovery (invited talk)
F.J. Luque.

Universidad Europea de Madrid (Spain)
Celebration date (format: 19/05/2023)

Molecular Dynamics: From motion of atoms to biomolecular function and molecular design.
F.J. Luque.

4th Annual Tomorrow Tastes Mediterranean Conference
Barcelona (Espanya)
Celebration date (format: 27/11/2023)

Computational gastronomy and the use of AI as a tool for culinary and nutritional research
Axel Bidon-Chanal Badia

Science & Cooking World Congress Barcelona 2023
Barcelona (Espanya)
Celebration date (format: 11-13/11/2023)

Formació en processos cientifico-gasronòmics
Davide Cassi, Axel Bidon-Chanal Badia

18th Annual Congress of International Drug Discovery Science and Technology
Amsterdam (Països Baixos)
Celebration date (format: 12-14/07/2023)

Revealing the molecular factors that govern the activation/inhibition AMPK mechanism by direct activators: towards a new drug design *(invited talk)*
C. Estarellas.

XVIII Iberian Peptide Meeting
Sesimbra (Portugal)
Celebration date (format: 27/11/2023)

Design and synthesis of novel hemagglutinin fusion peptide inhibitors of H1N1 influenza virus (talk)
de la Cruz, A.; de Castro, S.; Rimaux, S.; Stevaert, A.; Naesens, L.; Hermoso-Pinilla, F. J.; Ginex, T.; Luque, F. J.; Camarasa, M. J.; Velázquez, S.

Data science in biophysics for applications to drug discovery.
CECAM – Online
Celebration date (23/03/2023)

Towards the understanding of enzymatic mechanism of AMPK by specific modulators of β-isoforms (poster)
Barmpidi, K.; Luque, F.J.; Estarellas, C.

9th ESWI Influenza Conference 2023
Valencia (Spain)
Celebration date (17-20/09/2023)

A novel class of influenza virus fusion inhibitors with strong activity against H1 hemagglutinin and a similar binding pocket as arbidol (poster)
Rimaux, S.; Martín, J.; Valdivia, A.; Stevaert, A.; Luque, F. J.; Vázquez, S.; Naesens, L.

10th International BSC Severo Ochoa Doctoral Symposium
Barcelona (Spain)
Celebration date (02/05/2023)

Ranking allosteric activators of AMPK by absolute binding free energy calculations with fun-metad (poster)
Evans, R.; Luque, F.J.; Estarellas, C.

VIII SEQT Summer School. Medicinal Chemistry and Chemical Biology in drug discovery: The Pharma perspective
Santiago de Compostela (Spain)
Celebration date (19-21/06/2023)

Novel trimeric fusion inhibitors of hemagglutinin of influenza virus H1N1
De la Cruz, A.; De Castro, S.; Naesens, L.; Luque, F. J.; Camarasa, M. J.; Velázquez, S.
Computer-aided drug design of hemagglutinin fusion peptide inhibitors (poster)
Hermoso-Pinilla, F. J.; Velázquez, S.; Camarasa, M. J.; Ginex, T.; Luque, F. J.
Towards a new strategy for fighting Mycobacterium tuberculosis through the reductase-trHbN complex(poster)
Barmpidi, K.; Estarellas, C.; Luque, F. J.

IX SEQT Young Research Symposium
Santiago de Compostela (Spain)
Celebration date (22/06/2023)

Unravelling the molecular factors of isoform selectivity in AMPK by small molecules (poster)
Barmpidi, K.; Luque, F. J.; Estarellas, C.

2023 #RSCPoster Twitter Conference
Cambridge (Regne Unit), Virtual
28/Febrer/2023

Functionalization of Alkenes with Copper(I) to Obtain Fluorinated Alcohols (pòster)
F. A. Gómez-Mudarra, G. Aullón, J. Jover

62nd Sanibel Symposium
Bonita Springs (Florida, EUA)
10-13/Març/2023

Theoretical Challenges in Molecular Magnetism and Spintronics (conferència invitada)
E. Ruiz

9th EFEPR school
Ginebra (Suïssa)
3-9/Setembre/2023

Encapsulation of Metallocenes in Cucurbit[n]urils (pòster)
A. Silvestre-Llora, S. Gómez-Coca, E. Ruiz
Spin Relaxation of Ferrocenium Encapsulated in alpha-Cyclodextrin (pòster)
S. Gómez-Coca, A. Silvestre-Llora, M. Amoza, E. Ruiz

XXV Conference on Organometallic Chemistry (EuCOMC XXV)
Alcalá de Henares (Espanya)
4-8/Setembre/2023

Synthesis, Structure and Properties of Low-Valent Monocyclopentadienylchromium Hydride Complexes *(pòster)*
A. Calvo-Molina, J. Jover, A. Pérez-Redondo, C. Yélamos

Emerging Research on Molecule-Based Magnets: from Theory to Experiment
Guangzhou (China)
7-9/Setembre/2023

Controlling Slow Spin Relaxation by Encapsulation (conferència invitada)
E. Ruiz

18th International Conference on Molecule-based Magnets (ICMM2023)
Nanjing (China)
10-14/Setembre/2023

From Single-Molecule to 2D Layers: Magnetism and Transport (conferència invitada)
E. Ruiz

LatinXChem
Virtual (X/Twitter)
16-17/Octubre/2023

Cu(I)-catalyzed Synthesis of Fluorinated Alcohols from Alkenes and Ketones: DFT Studies (pòster)
F. A. Gómez-Mudarra, J. Jover, G. Aullón

VI Tesimarató de Química
Barcelona (Espanya)
21/Novembre/2023

Transició Sostenible: Explorant Alternatives als Metalls Preciosos en Catàlisi Homogenea (comunicación oral)
F. A. Gómez-Mudarra, J. Jover, G. Aullón

From Bioinorganic Chemistry to Catalysis (4th Edition)
Polymat, San Sebastian, Spain
12-05-2023

Supramolecular materials with life-like functions (Invited talk)
Mohit Kumar

Molecules confined in helium nanodroplets - new light sources for new materials and new applications. Hybrid COSY meeting
Praga (Czech Republic)
16 June 2023

On the dynamics of photodissociation and vibrational relaxation of diatomics in HeNDs (talk)
M. González

Seminaris del Institut Català de Nanociència y Nanotecnologia (ICN2)
Bellaterra (Spain)
12/12/2023

Computational Assessment of MXenes Bandgap Engineering for the Photocatalytic Water Splitting (Invited speaker)
F. Viñes

Erasmus Mundus Master in Sustainable Chemistry
Université de Poitiers, Poitiers (France)
01/12/2023-02/12/2023

Computational Methods and Models in Modern Heterogeneous Catalysis - Vols. I-IV (Invited speaker)
F. Viñes

Seminarios de la Universidad de Medellín
Medellín (Colombia)
31/11/2023

Surface Modelling for Energy & Sustainabiliy Applications (Invited speaker)
F. Viñes

8th International Conference on Semiconductor Photochemistry (SP8)
Strasbourg (France)
11/09/2023-15/09/2023

Computational Study of MXenes as Photocatalytic Materials (Oral Flash Communication)
D. Ontiveros
Computational Study of MXenes as Photocatalytic Materials (Poster)
D. Ontiveros

European Material Research Society
Strasburg, France
05/06/2023

Charge Reservoirs in an Expanded Halide Perovskite Analog: Enhancing High-Pressure Conductivity through Redox-Active Molecules.
Matheu, R.; Umeyana, D.; Karunadasa, H.

Triennial Congress of the World Association of Theoretical and Computational Chemists Applications (WATOC 2022)
Vancouver (Canada)
03/07/2023-08/07/2023

Grazynes: Carbon-Based 2D Composites with Exotic Properties and Applications (Oral Communication)
P. Gamallo

Workshop on kMC as a Tool for Understanding Catalytic Function
Fritz-Haber Institute, Berlin (Germany)
08/05/2023-10/05/2023

Effect of Terminations on the Hydrogen Evolution Reaction Mechanism on Ti_3C_2 MXene (Poster)
L. Meng
Systematic Study of the Dissociation of CO Molecule on Transition Metal Surfaces (Poster)
D. Vázquez-Parga

Computational Seminars at the School of Chemistry
Cardiff (United Kingdom)
12/04/2023

Stability of Photoactive TiO_2 Nanoparticles in Water Environment (Invited Lecturer)
Á. Morales-García

International Workshop & NIS colloquium (Photo)catalysts for sustainable fuel production
Turin (Italy)
21/09/2023

Realistic Photoactive TiO_2 Nanoparticles: A trip from Anhydrous to Hydrated Environments (Invited Speaker)
Á. Morales-García

XIV Congreso Internacional de Docencia e Investigación en Química
Ciudad de Méjico (Méjico)
07/07/2023

El futuro de la química computacional (Invited Speaker)
Á. Morales-García

Research Stays in Recognized Centers

Petr Jurečka

Palacký University Olomouc, Olomouc (Czech Republic)
Carles Eduard Curutchet Barat, University of Barcelona
February 2023

Petr Jurečka

Palacký University Olomouc, Olomouc (Czech Republic)
Renato Dias da Cunha, University of Barcelona
February-April 2023

Elena Cubero

Gain Therapeutics, Barcelona (Spain)
Özge Ergün, University of Barcelona
February-April 2023

Marco Cecchini

University of Strasbourg, Strasbourg (France)
Özge Ergün, University of Barcelona
September-December 2023

Maria João Ramos

University of Porto, Porto (Portugal)
Gül Beste Özaydin, University of Barcelona
November 2023 – January 2024

Jörg Libuda

Friedrich-Alexander Universität Erlangen-Nürnberg, Erlangen (Germany)
Konstantin Neyman
March-April 2023

Prof. Maria Ibañez

Institute of Science and Technology Austria (ISTA), Wien, Austria

Josep Puigmartí-Luis, UB

March 2023

Dr. Ciao Xiaobao

Guangzhou Laboratory, Guangzhou, China
Josep Puigmartí-Luis, UB

June 2023

Dr. Xiaobao Cao

International Biological Island, Guangzhou, China

Josep Puigmartí-Luis, UB
August 2023

Prof. Zuobin Wang

Changchun University of Science and Technology (CUST), Changchun, China

Josep Puigmartí-Luis, UB
December 2023

Prof. Xiangzhong Chen

Fudan University, Shanghai, China

Josep Puigmartí-Luis, UB
December 2023

Prof. Filippo Coletti

ETH Zurich, Zurich, Switzerland

Josep Puigmartí-Luis, UB
December 2023

Prof. Fabio Petrucci

Sorbonne University, Paris (France)

Beatriz Piniello Castillo, Universitat de Barcelona

April to June 2023

Prof. Elisa Fadda

Maynooth University, Maynooth (Ireland)

Irene Cuxart Sánchez, Universitat de Barcelona

March to May 2023

Dra. Rocío Mercado Oropeza

Chalmers University of Technology, Göteborg (Sweden).

Mª Nuria Peralta Moreno, IQTC-UB.

From October 2023 to February 2024

Michael Nolan

Tyndall Institute, Cork (Ireland)

Miquel Allès Coll, University of Barcelona

February-May 2023

Participation in Competitive Funded Research Projects

ALLODD - Allostery in Drug Discovery.
Carles Curutchet, Xavier Barril & Jordi Juárez, Universitat de Barcelona
H2020-MSCA-ITN-2020 Project 956314, 2021-2025
Financing entity (EU)
Amount: 454,049.76 €

Modelling the interplay between structure and spectroscopy in biosystems.
Carles Curutchet, Universitat de Barcelona
PID2020-115812GB-I00, 2021-2024
Financing entity (MINECO)
Amount: 96,800 €

Computational Biology and Drug Design.
F. Javier Luque, Universitat de Barcelona
2021SGR00671, 2022-2025
Financing entity (GENCAT)
Amount: 40,000 €

Interacciones no-covalentes en macromoléculas de ADN no-naturales y clústeres de boro.
Jordi Poater, Universitat de Barcelona
PID2022-138861NB-I00, 2023-2026
MINECO
Amount: 125.000 €

Laboratori de Materials Inorgànics i Catàlisi / LMI.
Rosario Núñez, ICMAB
2021SGR442, 2021-2024
GENCAT
Amount: 40.000 €

Computational modelling of complex materials for advanced technologies
P. Alemany, K. Neyman, Universitat de Barcelona
PID2021-128217NB-I00, 2022-2025
MCIUN
108900€

Computational modelling of complex materials for advanced technologies
Bruix, Universitat de Barcelona
PID2022-140120OA-I00, 2023-2026
MCIUN

Excellence in colloid and interface research & innovations for better quality of life
K. Neyman (PI for UB), Universitat de Barcelona
Networking project "EXTREME", 2021-2024
Bulgarian Ministry of Education and Science
0€

Recognized research "Grup d'Estructura Electrònica"
P. Alemany, Universitat de Barcelona
2021SGR00286, 2022-2024
Generalitat de Catalunya
40000€

Pre-doctoral FPI grant for Pablo Castro Latorre
K. Neyman, Universitat de Barcelona
PRE2019-088979, 2021-2025
MICIN
98250€

Pre-doctoral FPI grant for Riccardo Farris
K. Neyman, Universitat de Barcelona
PRE2020-091903, 2021-2025
MICIN
98960€

OPen-shell ELectronic SYStems (OPELSYS).
Mercè Deumal Solé, Universitat de Barcelona
2021SGR00354, 2022-2024
GENCAT
Amount: 40.000 €

Multiscale computational study of the catalytic conversion of greenhouse gases and hydrogen production through functionalized zeolites
Principal Investigator(s), Pablo Gamallo Belmonte / Ramon Sayós Ortega. Universitat de Barcelona
PID2022-138180OB-I00, 01/09/2023 - 31/08/2026
Financing entity (MINECO, EU, GENCAT,...): Ministerio de Ciencia e Innovación
Amount: 118.750,00 €

A paradigm shift for the future's thermal management devices through radical innovation in new materials and additive manufacturing (ThermoDust).
Principal Investigator(s), Dr. Sergi Dosta Parras. Universitat de Barcelona
101046835, 01/11/2022 - 31/10/2026
Financing entity (MINECO, EU, GENCAT,...): EUUN - Unió Europea
Amount: 656.796,00 €

Càtedra UB AmesPore
Principal Investigator(s), Dr. Juan Llorens Llacuna. Universitat de Barcelona
2020 - 2023
Financing entity (MINECO, EU, GENCAT,...): AMES Sinteric Metallic Components
Amount: 60.000 €

Mención de Excelencia Maria de Maetzu al Institut de Química Teòrica i Computacional Principal Investigator(s), Dr. Eliseo Ruiz Sabin. Universitat de Barcelona
CEX2021-001202-M, 01/01/2023 - 31/12/2026
Financing entity (MINECO, EU, GENCAT,...): MEICO - Ministerio de Economia, Industria y Competitividad
Amount: 2.000.000 €

Autoensamblaje disipativo de materiales supramoleculares porosos basados en cajas metal-orgánicas (DISSPORMAT).
A. Sorrenti, Universitat de Barcelona
CNS2023-145154 (Consolidación Investigadora 2023) 2024-2026
Ministerio de Ciencia e Innovación
Amount: 199.583 €

Solvent Recovery from waste generated during Liposome production (SolReLip).
A. Sorrenti, Universitat de Barcelona
311993 2022-2023
Laboratorios Reig-Jofre, S.A., R&D project with a Company
Amount: 34.000 €

Síntesis y crecimiento controlado de estructuras metal-orgnaicas porosas con tecnologías microfluidicas
J. Puigmartí Luis, Universitat de Barcelona
PID2020-116612RB-C33 2021-2024
Ministerio de Ciencia e Innovación
Amount: 177.500 €

Magnetoelectric 3D printing technology - the revolution of actuatable composites (EVA),
J. Puigmartí Luis, Universitat de Barcelona
101047081 (EIC Pathfinder Open 2021) 2022-2026
European Union
Amount: 629.875 €

ChemInFlow Group (Chemistry In Flow and Nanomaterials Synthesis Group)
J. Puigmartí Luis, Universitat de Barcelona
SGR-Cat 2021 SGR 00270 2022-2025
AGAUR
Amount: 36.000 €

Ultra-versatile Structural PRINTing of amorphous and tuned crystalline matter on multiple substrates (SPRINT)
J. Puigmartí Luis, Universitat de Barcelona
801464 2020-2023
AGAUR
Amount: 261.173,51€

European metal-organic framework network: combining research and development to promote technological solutions' (EU4MOFs).
Prof. Stefan Wuttke, Prof. Puigmartí-Luis (Management Committee) (UB)
CA22147, 2023 - 2027
COST Action
680.000 €

EVA: ME 3D printing technology – the revolution of actuatable composites
Prof. J. Puigmartí-Luis, UB
I1RN002262 EVA (101047081), 2022 – 2026
HORIZON-EIC-2021-PATHFINDEROPEN-01
2,109,624 €

MAgnetically steerable wireless Nanodevices for the tarGeted delivery of therapeutIc agents in any vascular rEgion of the body (ANGIE)
Prof. Salvador Pané (ETH Zurich), Prof. J. Puigmartí-Luis is the project leader at UB
402185 (952152), 2021 - 2024
European Commission; FET PROACTIVE; Call: H2020-EIC-FETPROACT-2019
4,000,000.00 € from where 550,000.00 € to University of Barcelona (UB)

Grup de recerca consolidat: Estructura i funció en macromolècules
C. Rovira (Universitat de Barcelona), I. Fita (CSIC de Barcelona)
2021SGR-00680, 2022 – 2025
GENCAT (AGAUR)
Amount: 60.000,00 €

Computer simulation of catalytic mechanisms in glycoprocessing enzymes by means of QM/MM molecular dynamics techniques
C. Rovira (Universitat de Barcelona)
PID2020-118893GB-100 – Compglyco, 2021-2024
MICINN
Amount: 120.000,00 €

Activity-Based Profiling of Glycoprocessing Enzymes for Human Health and a Sustainable Society
G. J. Davies (University of York, United Kingdom), H. S. Overkleeft (Universiteit Leiden, The Netherlands), C. Rovira (Universitat de Barcelona)
ERC-2020-SyG-951231- Carbocentre, 2021-2027
EU
Amount (corresponding to UB): 1.578.800,00 €

Nuevas estrategias computacionales para el estudio de agregación y adsorción de microplásticos y nanoplásticos a contaminantes en medios acuáticos naturales
Barazorda Ccachuana, Haruna Luz
151-2020-FONDECYT, 2020-2023
45.550€

Uso de nuevas técnicas computacionales de modelamiento a multiescala para la determinación de los mecanismos de adsorción de ácidos húmicos a lixiviados de microplásticos
Francesc Mas Pujadas
VRINVFMP003-POP-092022, 2023-2025
24.000€

Computational design of photoactive molecular materials for optoelectronic applications.
Maria Fumanal, Universitat de Barcelona
PID2022-140460NA-I00, 2023-2027
Financing entity: MINECO
Amount: 101.250,00 €

Open-shell molecule-based materials: understanding and predicting structure and physical properties through computational modeling
Jordi Ribas (IP1), Mercè Deumal (IP2), Universitat de Barcelona
PID2020-117803GB-I00, 2021-2024
Financing entity: MINECO
Amount: 121.000,00 €

Computational modelling of the structures, properties and electroreactivity of electrodes functionalised with electroactive molecules
Stefan Bromley (IP), Universitat de Barcelona
TED2021-132550B-C21, 2023-2024
Financing entity: MICIU
Amount: 132.480,00 €

Tuning Tubulin Dynamics and Interactions to Face Neurotoxicity: a Multidisciplinary Approach for Training and Research (TubInTrain).
IP: Marta Cascante Serratosa, Universitat de Barcelona
860070, 01/10/2019- 30/09/2023
EUUN - Unió Europea
426.209,76 €

Molécula activadora de la señalización de kras oncogénico como terapia dirigida contra el cáncer colorectal.
IP: Nieves Agell Jane, Universitat de Barcelona
NBME, PDC2022-133653-I00, 01/12/2022- 30/11/2024
W0122 - Ministerio de Ciencia e Innovación
149.500,00 €

SGRC - Ajuts de Suport als Grups de Recerca de Catalunya (SGR)
IP: Marta Cascante Serratosa, Universitat de Barcelona
2021 SGR 00350/ 01/01/2022- 30/06/2025
Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR)
60.000,00 €

Master Evaluation and Material Transfer Agreement
Investigadores responsables: Nieves Agell Jane / Eduardo Garrido Sagarzazu / Jaime Rubio Martinez / Baraa Abuasaker / Sonia Brun Lozano / Montserrat Jaumot Pijoan / Marta Vilaplana Saiz / Maria Pujol Dilme
KNOW-Contractes d'explotació de know-how. Royalties o derivats de cesió de llicència/patent/know-how. 06/06/2023- 05/06/2027
Entidad Financiadora: ValiRx PLC

Synthetic Neurons and Artificial Photoactivated Synapses
Bart Limburg, Universitat de Barcelona
G.A. 101076014, 2023-2027
EU ERC-StG
Amount: €1 688 047

Next-Generation Photocatalysts to Enhance Quantum Yields in Organic Synthesis
Bart Limburg, Universitat de Barcelona
CNS2023-144535, 2024-2025
MICINN - Incentivación de la consolidación investigadora
Amount: € 199 999

Explorando nuevas estrategias en enfermedades víricas y tuberculosis: Plasticidad conformacional, resistencia a mutaciones y modificación química pseudoirreversible.
F. J. Luque, Universitat de Barcelona
PID2020-117646RB-I00, 2021-2024
Ministerio de Ciencia e Innovación (MICINN)
Amount: 170.610,00 €

Iterative experimental and computational approach to modulate bioactive leptin peptides towards novel therapeutic strategies for Alzheimer's disease.
C.Pubill, C.Estarellas, Universitat de Barcelona
PID2022-142623OA-I00, 2023-2026
Ministerio de Ciencia e Innovación (MICINN)
Amount: 106.250,00 €

Towards an improvement in diagnostics and treatment strategies for TB control (ADVANCE- TB)
PI: Alicia Lacoma, Institute Germans Trias – Hospital Can Ruti
Cost Action 21164, 2022 - 2026
European Union
Amount granted: €

Development of virtual screening activities aimed to the identification of active compounds directed to validated targets through Computational Chemistry
PI: F.J. Luque, C. Estarellas, University of Barcelona
FBG 311918, 2022 - 2023
Université Libre de Bruxelles
Amount granted: 12.683,00 €

Serveis en Química Computacional
F.J. Luque, C. Estarellas, University of Barcelona
FBG 310755, 2020 - 2023
Pharmacelera S.A.
Amount granted: 101.289,49 €

Inteligencia Artificial para Dispositivos Magnéticos en Computación Cuántica y Neuromórfica.
Eliseo Ruiz, Universitat de Barcelona
ED2021-129593B-I00, 2022-2024
Ministerio de Ciencia e Innovación

Estructura electrónica y propiedades físicas de moléculas y sólidos inorgánicos.
Eliseo Ruiz, Universitat de Barcelona
PID2021-122464NB-I00, 2022-2025
Ministerio de Ciencia e Innovación

MATERIALES BLANDOS QUIMICAMENTE ALIMENTADOS CON FUNCIONES SIMILARES A SISTEMAS VIVOS
Mohit Kumar, Universitat de Barcelona
PID2021-126244NA-I00, 2022-2025
MINECO
75.020 €

Computational Materials Science Laboratory (CMSL) / Laboratori de Ciència de Materials Computacional
Francesc Illas, Universitat de Barcelona
2021SGR79, 2022-2024
Generalitat de Catalunya
60.000€

Atom-Dispersed Catalysts for the Thermo-Photo Valorization of CO2: Experimental Design and Computational Modeling
Francesc Illas & Francesc Viñes, Universitat de Barcelona
TED2021-129506B-C22, 2022-2024
Ministerio de Ciencia e Innovación
169.510€

Computationally assisted optimization of new two-dimensional MXene catalysts for greenhouse gas reduction and hydrogen generation
Francesc Viñes and Carmen Sousa, Universitat de Barcelona
PID2021-126076NB-I00, 2022-2025
Ministerio de Ciencia e Innovación
169.400€

Excited states Dynamics of TiO_2 nanostructures: Towards engineering enhanced photocatalytic activity under sunlight
Ángel Morales-García, Universitat de Barcelona
PID2020-115293RJ-I00, 2022-2025
Ministerio de Ciencia e Innovación
45.530€

Roc Matheu, Universitat de Barcelona
PID2022-137777NA-I00
Agencia Estatal de Investigación
106 250 €

Institut de Química Teòrica i Computacional