Institut de Química Teòrica i Computacional

EXCELENCIA MARÍA DE MAEZTU

UNIVERSITAT DE BARCELONA

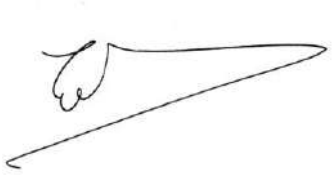
Institut de Química Teòrica i Computacional de la Universitat de Barcelona (IQTCUB)

Activity Report 2022

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

I. IQTCUB OVERVIEW

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

I.1 DIRECTION TEAM

The IQTCUB direction team during 2022 has been:

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

I.2 IQTCUB RESEARCH LINES

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

1. **Clean and sustainable energy**

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

2. Nanomaterials and nanoelectronics

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

3. Biomedicine and Soft Matter

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

I.3 IQTCUB MEMBERS

IQTCUB involves a total of 121 professors and researchers: The full list of members of IQTCUB (including the corresponding academic situation and affiliation within UB) is provided below.

Family Name	Name	Nationality (Gender)	Depart./Unit (Section)
Full Professors			
Aguilar Navarro	Antonio	SPAIN (M)	Materials Science & Physical Chemistry
Alemany i Cahner	Pere	SPAIN (M)	Materials Science & Physical Chemistry
Álvarez Reverter	Santiago	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
Aullón López	Gabriel	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
Bofill Villà	Josep Maria	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
Curutchet Barat	Carles E.	SPAIN (M)	Pharm. & Pharm. Tech. & Phys. Chem.
Deumal Solé	Mercè	SPAIN (F)	Materials Science & Physical Chemistry
González Pérez	Miguel	SPAIN (M)	Materials Science & Physical Chemistry
Illas Riera	Francesc	SPAIN (M)	Materials Science & Physical Chemistry
Luque Garriga	Francisco J.	SPAIN (M)	Nutrition, Food Sciences & Gastronomy
Mas Pujadas	Francesc	SPAIN (M)	Materials Science & Physical Chemistry

Novoa Vide	Juan José	SPAIN (M)	Materials Science & Physical Chemistry
Reigada Sanz	Ramón	SPAIN (M)	Materials Science & Physical Chemistry
Rubio Martínez	Jaime	SPAIN (M)	Materials Science & Physical Chemistry
Ruiz Sabin	Eliseo	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
Sayós Ortega	Ramón	SPAIN (M)	Materials Science & Physical Chemistry
Sousa Romero	Carme	SPAIN (F)	Materials Science & Physical Chemistry

Associate Professors

Costa Sala	Ramón	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
D. P. Ribeiro Moreira	Iberio	SPAIN (M)	Materials Science & Physical Chemistry
Giménez Font	Xavier	SPAIN (M)	Materials Science & Physical Chemistry
Huarte Larrañaga	Fermín	SPAIN (M)	Materials Science & Physical Chemistry
Lucas Alcorta	Josep Maria	SPAIN (M)	Materials Science & Physical Chemistry
Llunell Marí	Miquel	SPAIN (M)	Materials Science & Physical Chemistry
Mota Valeri	Fernando	SPAIN (M)	Materials Science & Physical Chemistry
Paniagua Valle	Juan Carlos	SPAIN (M)	Materials Science & Physical Chemistry
Solé Sabaté	Albert	SPAIN (M)	Materials Science & Physical Chemistry
Vilaseca Font	Eudald	SPAIN (M)	Materials Science & Physical Chemistry

Other Categories (Professors Agregats)

Bidon-Chanal Badia	Axel	SPAIN (M)	Nutrition, Food Sciences & Gastronomy
Bonet Ruiz	Jordi	SPAIN (M)	Chem. Engineering & Analytical Chem.
Gamallo Belmonte	Pablo	SPAIN (M)	Materials Science & Physical Chemistry
Madurga Díez	Sergio	SPAIN (M)	Materials Science & Physical Chemistry
Plesu Popescu	Alexandra	SPAIN (F)	Chem. Engineering & Analytical Chem.
Ribas Ariño	Jordi	SPAIN (M)	Materials Science & Physical Chemistry
Viñes Solana	Francesc	SPAIN (M)	Materials Science & Physical Chemistry

ICREA Research Professors

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

Other Categories (Professors Lectors)

Estarellas	Carolina	SPAIN (F)	Nutrition, Food Sciences & Gastronomy
Gómez Coca	Silvia	SPAIN (F)	Inorganic Chemistry & Organic Chemistry
Jover Modrego	Jesús	SPAIN (M)	Inorganic Chemistry & Organic Chemistry

Juárez Jiménez	Jordi	SPAIN (M)	Pharm. & Pharm. Tech. & Phys. Chem.
Morales Garcia	Ángel	SPAIN (M)	Materials Science & Physical Chemistry
		SPAIN (F)	Chem. Engineering & Analytical Chem.

Other Categories (Professors Associats)

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

Postdoctoral contracts

Beatriu de Pinós-Juan de la Cierva

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

Ramón y Cajal

Calle Vallejo	Federico	COLOMBIA (M)	Materials Science & Physical Chemistry
Cortijos Aragonès	Albert	SPAIN (M)	Materials Science & Physical Chemistry
Cirera Fernández	Jordi	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
Echeverría López	Jorge	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
Fumanal Quintana	Maria	SPAIN (F)	Materials Science & Physical Chemistry
Guix Noguera	Maria	SPAIN (F)	Materials Science & Physical Chemistry

Contracte Projecte de Recerca

Alonso Benito	Gerard	SPAIN (M)	Materials Science & Physical Chemistry
Belce	Yonca	TURKEY (F)	Materials Science & Physical Chemistry
Calvelo Souto	Martín	SPAIN (M)	Inorganic Chemistry and Organic Chem.
Garcia Cirera	Beltzane	SPAIN (M)	Materials Science & Physical Chemistry
López Marne	Estefania	SPAIN (F)	Materials Science & Physical Chemistry
Mattera	Michele	ITALY (M)	Materials Science & Physical Chemistry
Nin Hill	Alba	SPAIN (F)	Inorganic Chemistry & Organic Chemistry
Nicholas	James	UK (M)	Materials Science & Physical Chemistry
Rodríguez Remesal	Elena	SPAIN (F)	Materials Science & Physical Chemistry
Rodríguez San Miguel	David	SPAIN (M)	Materials Science & Physical Chemistry

Sorrenti	Alessandro	ITALY (M)	Materials Science & Physical Chemistry
Sun	Xiaobo	CHINA (M)	Inorganic Chemistry & Organic Chemistry

Other

Albareda Piquer	Guillem	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
Blanco Andrés	Pablo Miguel	SPAIN (M)	Materials Science & Physical Chemistry
Herrera Restrepo	Ramón S.	COLOMBIA (M)	Materials Science & Physical Chemistry
Kolb	Manuel	GERMANY (M)	Materials Science & Physical Chemistry
Liao	Qinghua	CHINA (M)	Inorganic Chemistry & Organic Chemistry
Llauradó Capdevila	Gemma	SPAIN (F)	Materials Science & Physical Chemistry
López Suarez	Miquel	SPAIN (M)	Materials Science & Physical Chemistry
Macià Escatllar	Antoni	SPAIN (M)	Materials Science & Physical Chemistry
Matheu	Roc	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
Ngo	Tuan	VIETNAM (M)	Materials Science & Physical Chemistry
Nguyen	Thao	VIETNAM (F)	Materials Science & Physical Chemistry
		SPAIN (F)	Inorganic Chemistry & Organic Chemistry
Vilà Casanovas	Arnau	SPAIN (M)	Materials Science & Physical Chemistry

Ph.D. Students

Beca Programa María de Maeztu

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

FI Grant (Catalan Government Program)

Aledavood	Elnaz	SPAIN (F)	Nutrition, Food Sciences & Gastronomy
García-Romeral	Néstor Mauricio	SPAIN (M)	Materials Science & Physical Chemistry
Mariñoso Guiu	Joan	SPAIN (M)	Materials Science & Physical Chemistry
Martín Rodríguez	Alejandro	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
Ozaydin	Gül Beste	TURKEY (F)	Pharm. & Pharm. Tech. & Phys. Chem.
Piniello Castillo	Beatriz	SPAIN (F)	Inorganic Chemistry & Organic Chemistry
Vega Domínguez	Lorena	SPAIN (F)	Materials Science & Physical Chemistry

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

Almacellas Salillas	David	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
Bernuz Fitó	Efrem	SPAIN (M)	Materials Science & Physical Chemistry
Cánovas Montes	Manuel Ant.	SPAIN (M)	Materials Science & Physical Chemistry

Castro Latorre	Pablo	CHILE (M)	Materials Science & Physical Chemistry
Cuxart Sánchez	Irene	SPAIN (F)	Inorganic Chemistry & Organic Chemistry
Esquivias Baut. Lisb.	Oriol	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
Farris	Riccardo	ITALY (F)	Materials Science & Physical Chemistry
Gómez Mudarra	Francisco A.	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
Piñero Vargas	Juan José	SPAIN (M)	Materials Science & Physical Chemistry
Piqué Caufapé	Oriol	SPAIN (M)	Materials Science & Physical Chemistry
Recio Poo	Miguel	SPAIN (M)	Materials Science & Physical Chemistry
Regalado Aguilar	Mauricio	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
Rivas Fernández	José Pablo	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
Romeo	Eleonora	ITALY (F)	Materials Science & Physical Chemistry
Santiago Piera	Raúl	SPAIN (M)	Materials Science & Physical Chemistry

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

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

ITN UE Grant

Mnevets	Daniil	BELARUS (M)	Inorganic Chemistry & Organic Chemistry

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

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

Beca Doctorat Industrial

Campos-Vicens	Lluis	SPAIN (M)	Pharm. & Pharm. Tech. & Phys. Chem.
Troyano Ferré	Carles	SPAIN (M)	Chem. Engineering & Analytical Chem.

Other

Barazorda-Ccahuana	Haruna	PERU (F)	Materials Science & Physical Chemistry
Barmpidi	Aikaterini	GREECE (F)	Nutrition, Food Sciences & Gastronomy
Cabello Gallego	Ruben	SPAIN (M)	Chem. Engineering & Analytical Chem.
Calzada Escrig	Adrià	SPAIN (M)	Materials Science & Physical Chemistry
Campos-Vicens	Lluís	SPAIN (M)	Nutrition, Food Sciences & Gastronomy

Colomer Llombart	Eduard	SPAIN (M)	Materials Science & Physical Chemistry
De Donato Pérez	Andreu Avel·lí	SPAIN (M)	Materials Science & Physical Chemistry
Dolz García	Daniel	SPAIN (M)	Materials Science & Physical Chemistry
Ergün	Özge	TURKEY (F)	Pharma., Pharmac. Tech & Phys. Chem.
De Oliveira Almeida	Michell	BRASIL (M)	Materials Science & Physical Chemistry
Figueras Valls	Marc	SPAIN (M)	Materials Science & Physical Chemistry
García Gonzalo	Lluc	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
Gil	Diego	ARGENTINA (M)	Inorganic Chemistry & Organic Chemistry
Gracia Gil	Alejandro	SPAIN (M)	Materials Science & Physical Chemistry
Jurado Mañas	Anabel	SPAIN (M)	Materials Science & Physical Chemistry
Morales Salvador	Raúl	SPAIN (M)	Materials Science & Physical Chemistry
		SPAIN (M)	Materials Science & Physical Chemistry
Meng	Ling	CHINA (M)	Materials Science & Physical Chemistry
De Moya Valenzuela	Natalia	SPAIN (F)	Materials Science & Physical Chemistry
			Materials Science & Physical Chemistry
Pepe	Alessandro	ITALY (M)	Inorganic Chemistry & Organic Chemistry
Peralta Moreno	Maria Nuria	SPAIN (M)	Materials Science & Physical Chemistry
Quinlivan Domínguez	Jon Eunan	SPAIN (M)	Materials Science & Physical Chemistry
Rivas Fernández	José Pablo	SPAIN (M)	Inorganic Chemistry & Organic Chemistry
Roncero Barrero	Cristina	SPAIN (F)	Materials Science $ Physical Chemistry
Sağıroğlugil	Mert	TURKEY (M)	Inorganic Chemistry & Organic Chemistry
Saranjam	Leila	IRAN (F)	Materials Science & Physical Chemistry
Tarik	Karim	SPAIN (M)	Materials Science & Physical Chemistry
Urrego Ortiz	Ricardo	SPAIN (M)	Materials Science & Physical Chemistry
Valdivia	Aitor	SPAIN (M)	Nutrition, Food Sciences & Gastronomy
Vázquez Parga	David	SPAIN (M)	Materials Science & Physical Chemistry
Velasco	Arnau	SPAIN (M)	Materials Science & Physical Chemistry
Vidal Gironès	Oscar	SPAIN (M)	Inorganic Chemistry & Organic Chemistry

I.4 TECHNICAL STAFF

Apart from the academic and research personnel whose main activity is scientific research in theoretical and computational chemistry at IQTCUB, technical staff members take care of maintenance of the computational infrastructure and give support to the research groups. Their work is extremely important since they also implement the codes and optimize their performance.

Jordi Inglés Camats	*HPC System Administrator Manager*
Irene Zamora Carretero	*HPC System Administrator*
Begoña López Maestre	*Project Manager*
Patricia Verdugo Salomón	*3D Designer*
Aïda Valverde Sanchís	*Promoter*

I.5 EQUIPMENT

Currently, the IQTCUB computational facilities consist of nine calculation clusters located in two conditioned rooms of the Chemistry and Physics Faculty of UB. All the clusters except iqtc06 and iqtc07 are in a room near the garage of the faculty where it is cooled by two air conditioning machines of 47,000 and 66,000 KW, respectively. Iqtc06 and iqtc07 are located in a room called VAX, which is cooled by one air conditioner machine of 30,000 KW and another two of 9,000KW each.

CALCULATION CLUSTERS

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

lqtc11 (*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.

II. IQTCUB ACTIVITIES

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

Next, a description of activities and actions promoted by IQTCUB through 2022 is provided.

a. ***Research Start Help.*** This year the IQTCUB offered two postmaster grants to help students initiate a scientific career. Aikaterini Barmpidi and Daniel Dolz were the awarded students.

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

b. ***Scientific Dissemination Activities.*** The following scientific dissemination activities have been performed during 2022:

1. *"Synchronous Flipped Classroom in STEM subjects"*. X. Giménez, Revista de Educación ***391***, 15–39 (2021).
2. *"Pandèmia i Paràsits". X. Giménez,* Setmanari Montbui Journal 1924, 7 (2021).
3. *"Transición a las renovables: ya estamos en ello", X. Giménez, "*Entre Todos" section of El Periódico Journal, Pg 35, May 31st (2022).
4. *"(On–line) Active Learning and Digitalization in STEM subjects*: *a natural match*". Invited conference at **Istituto Politecnico di Milano**, Milano, Italy, 6/June/2022.

5. *"Active Learning @ University of Barcelona"*. Seminar at Education Innovation Working Group – Coimbra Group General Assembly. **University of Padova**, Padova, Italy, 8/June/2022.
6. *"Hybrid Physical and Virtual Spaces in the CHARM–EU Master*". Communication at Education Innovation Working Group Meeting – ***"From Learning Spaces to Learning Environments"***. University of Uppsala, Uppsala, Sweden, 9–10/Nov/2022.
7. *"SABER: fem possible un òptim rendiment acadèmic, en un entorn STEM"*. 9-hour **ICE course** at Universitat de Barcelona, Barcelona, 20–22/Jun/22.
8. *"Aprenentatge Actiu Basat en Problemes, Projectes o Reptes"*. 4–hour **ICE–IDP course** at Facultat de Psicologia, Universitat de Barcelona, 5/Jul/22.
9. *"Aprendizaje Activo Basado en Problemas, Proyectos o Retos*. 4–hour Special Seminar, Facultad de Química, Universidad de Vigo, 18–20/July/2022.

Divulgation seminars by Xavier Giménez:

1. *"UB s'Apropa 22".* INS Bellulla, Canovelles, 11/Jan/2022.
2. *"UB s'Apropa 22".* INS Milà i Fontanals, Vilafranca del Penedès, 12/Jan/2022.
3. *"UB s'Apropa 22".* INS Joan Oliver, Sabadell, 13/Jan/2022.
4. *"UB s'Apropa 22".* INS La Garrotxa, Olot, 18/Jan/2022.
5. *"UB s'Apropa 22".* Escola Educem II, Granollers, 19/Jan/2022.
6. *"UB s'Apropa 22".* INS Vil·la Romana, La Garriga, 20/Jan/2022.
7. *"UB s'Apropa 22".* INS Joan Oliver, Sabadell, 20/Jan/2022.
8. *"UB s'Apropa 22".* INS La Vall del Tenes, Sta. Eulàlia de Ronsana, 24/Jan/2022.
9. *"UB s'Apropa 22".* INS Pau Vila, Sabadell, 26/Jan/2022.
10. *"UB s'Apropa 22".* Escola Graví, Barcelona, 27/Jan/2022.
11. *"UB s'Apropa 22".* INS Bellulla, Canovelles, 27/Jan/2022.
12. *"UB s'Apropa 22".* INS Vinyet, Sitges, 28/Jan/2022.
13. *"UB s'Apropa 22".* INS Joan Brudieu, La Seu d'Urgell, 2/Feb/2022.
14. *"UB s'Apropa 22".* INS Rovira–Forns, Sta. Perpètua de Mogoda, 3/Feb/2022.
15. *"UB s'Apropa 22".* INS Rovira–Forns, Sta. Perpètua de Mogoda, 3/Feb/2022.
16. *"UB s'Apropa 22".* INS Moianès, Moià, 4/Feb/2022.
17. *"UB s'Apropa 22".* INS Moianès, Moià, 4/Feb/2022.
18. *"UB s'Apropa 22".* INS Joaquim Mir, Vilanova i la Geltrú, 10/Feb/2022.
19. *"UB s'Apropa 22".* Escola Daina–Isard, Olesa de Montserrat, 10/Feb/2022.
20. *"UB s'Apropa 22".* INS Pere Ribot, Vilassar de Mar, 18/Feb/2022.
21. *"UB s'Apropa 22".* INS Pere Ribot, Vilassar de Mar, 21/Feb/2022.
22. *"L'Aire que respirem".* **Toc–Toc UB Science Dissemination Program**, Escola Patronat Domènech, Barcelona, 22/Feb/2022.

23. *"L'Aire que respirem",* **Toc–Toc UB Science Dissemination Program,** Pla Comunitari La Verneda i La Pau, Barcelona, 24/Feb/2022.
24. *"UB s'Apropa 22".* INS Mollet, Mollet del Vallès, 2/Mar/2022.
25. *"UB s'Apropa 22".* INS La Roca, La Roca del Vallès, 3/Mar/2022.
26. *"UB s'Apropa 22".* INS La Roca, La Roca del Vallès, 3/Mar/2022.
27. *"UB s'Apropa 22".* INS Mollet, Mollet del Vallès, 4/Mar/2022.
28. *"La Màgia de l'aigua".* **Toc–Toc UB Science Dissemination Program**, Escola Patronat Domènech, Barcelona, 8/Mar/2022.
29. *"UB s'Apropa 22".* INS El Cairat, Esparreguera, 10/Mar/2022.
30. *"UB s'Apropa 22".* Escola Pia, Caldes de Montbui, 17/Mar/2022.
31. *"UB s'Apropa 22".* INS Lauro, Les Franqueses del Vallès, 24/Mar/2022.
32. *"UB s'Apropa 22".* INS Lauro, Les Franqueses del Vallès, 24/Mar/2022.
33. "*Llibres de Divulgació Científica*", **Màster de Comunicació Científica**, Univ. Barcelona, 30/Mar/2022.
34. *"La Màgia de l'Aigua"*, Conference at **Escola d'Adults Municipal El Roure Gros**, Caldes de Montbui, 8/Apr/2022.
35. *"L'origen dels elements químics".* **Toc–Toc UB Science Dissemination Program**, Institut Mercè Rodoreda, L'Hospitalet de Llobregat, 20/Apr/2022.
36. *"UB s'Apropa 22".* INS Argentona, Argentona, 22/Apr/2022.
37. *"Metales tóxicos, y sus efectos ambientales y sobre la salud humana"*, On–line Seminar, Biological Inorganic Chemistry course, **Universidad de Sevilla**, 26/Apr/2022.
38. *"L'Aire que Respirem".* 1st Conference in **Gaudir UB** course series, Universitat de Barcelona, 28/Apr/2022.
39. *"L'Aigua: la màgia de la substància més important".* 2nd Conference in **Gaudir UB** course series, Universitat de Barcelona, 5/May/2022.
40. *"De què estan fets els planetes i les estrelles?".* 3rd Conference in **Gaudir UB** course series, Universitat de Barcelona, 12/May/2022.
41. *"L'Hidrogen, una energia neta",* **Aules d'Extensió Universitària Delfí Dalmau i Argemir**, Caldes de Montbui, 18/May/2022.
42. *"L'energia que ens mou".* 4th Conference in **Gaudir UB** course series, Universitat de Barcelona, 26/May/2022.
43. *"Energies renovables: el futur serà net i sostenible*". 5th Conference in **Gaudir UB** course series, Universitat de Barcelona, 2/June/2022.
44. *"Els vehicles elèctrics*". 6th Conference in **Gaudir UB** course series, Universitat de Barcelona, 16/Jun/2022.

45. *"Els materials que ens envolten: l'evolució silenciosa cap a la modernitat*". 7th Conference in **Gaudir UB** course series, Universitat de Barcelona, 23/Jun/2022.
46. *"Millor i més petit impossible: les promeses dels motors moleculars*". 9th Conference in **Gaudir UB** course series, Universitat de Barcelona, 28/Jun/2022.
47. *"El Grafè: les promeses del material més revolucionari".* 10th Conference in **Gaudir UB** course series, Universitat de Barcelona, 30/Jun/2022.
48. *"La composició de la vida: la major part dels éssers vius compartim de què estem fets".* 10th Conference in **Gaudir UB** course series, Universitat de Barcelona, 7/July/2022.
49. *"La Màgia de l'Aigua"*, **Toc–Toc UB Science Dissemination Program, Institut Marta Mata**, Montornès del Vallès, 14/Nov/2022.
50. *"L'origen dels elements químics".* **Toc–Toc UB Science Dissemination Program**, **Institut Marta Mata**, Montornès del Vallès, 14/Nov/2022.
51. *"La Màgia de l'Aigua".* **Toc–Toc UB Science Dissemination Program, Institut Miquel Tarradell**, Barcelona, 16/Nov/2022.
52. *"Electricitat i Hidrogen, el futur net i sostenible".* STEAM project, Science Week. **Institut Guindàvols**, Lleida, 17/Nov/2022.

Other divulgation activities

- *VIII Festa de la Ciència de la UB*
  27-28/05/2022
  Pablo Gamallo

- *Fem Química al Laboratori*
  Gener 2022
  Pablo Gamallo

c. ***IQTCUB Meeting 2022.*** The event took place on July Tuesday 19th and Wednesday 20th. 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. Ryan G. Hadt from CalTech and Dr. Julien Michel from The University of Edimburgh. A poster session was held as well for this event.

d. ***Molecular Modelling: biomolecules and drug design 2022.*** From June 28th to July 1st, the summer computational school titled *Molecular Modelling: biomolecules and drug design 2022 took place.* Prof. Gabriel Aullón, 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)
-Enllaç i Estructura (G. Aullón and S. Gómez)
- Coarse-grained Molecular Dynamics simulations for soft-matter systems: from micelles to membranes (Ramón Reigada)
- Protein Molecular Dynamics (Carolina Estarellas and Salomé Llabrés)
- Visualising biomolecules in action (Matín Calvelo and José Pablo Rivas)
- Multi-scale modelling of solutions and biomolecules (Carles Curutchet)
- Drug Design (Jaime Rubio)
- Simulation of macromolecular systems (Sergio Madurga)

e. ***Computational Modelling: from Molecules to Materials 2022.*** From July 4th to July 9th, the summer computational school titled *Computational Modelling: from Molecules to Materials 2022* 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)

f. ***New Trends in Computational Chemistry 2022.*** This workshop was held on September 8th and 9th and it brought together worldwide leading experts in the application and development of Quantum Computing methods applied to atomistic modelling, hardware and software development.

Panel promoting the New Trends workshop.

g. ***Allosterism and Drug Discoveryh Conference.*** Event promoted by the ALLODD project (Allostery and Drug Discovery). Prof. Xavier Barril and Prof. Carles Curutchet groups participated in the workshop.

Program – Day 1 (13.06.2022)

09:00 – 09:05	Welcome
09:05 – 10:00	Plenary Talk – Allosterism: a historical perspective JP CHANGEUX, INSTITUT PASTEUR
10:00 – 10:45	Mapping the energetic and allosteric landscapes of protein binding domains BEN LEHNER, CRG
10:45 – 11:15	Coffee Break
11:15 – 12:00	To be announced
12:00 – 12:45	Different flavours of disorder seen by NMR: fuzzy complexes and breathing proteins MIQUEL PONS, UB
13:00 – 14:00	Lunch
14:00 – 14:45	Allosterism in GPCRs CHRIS DE GRAAF, SOSEI HEPTARES
14:45 – 15:30	Allosterism in Kinases FRANCESCO GERVASIO, UCL
15:30 – 16:00	Coffee Break
16:00 – 16:45	Allosterism and Drug Discovery: the merger of two worlds ZOE COURNIA, BRFAA
16:45 – 17:30	Drug-likeness, druggability and drug modalities XAVIER BARRIL, UB

Program – Day 2 (14.06.2022)

09:00 – 10:00	Allosterism in DNA MODESTO OROZCO, IRB
10:00 – 10:45	Computational investigation of allosteric mechanisms SILVIA OSUNA, UdG
10:45 – 11:15	Coffee Break
11:15 – 12:00	A role for allosteric sites in targeted protein degradation and E3 ligases CARLES GALDEANO, UB
12:00 – 12:45	An integrated platform for the discovery of peptidic ligands TBA, NOVO NORDISK
13:00 – 14:00	Lunch
14:00 – 14:45	Detection of secondary sites on proteins using fragment screening MARCEL VERDONK, ASTEX
14:45 – 15:30	To be announced
15:30 – 16:00	Coffee Break
16:00 – 17:00	Present & future of Allosteric drug discovery ROUND TABLE
17:00 – 17:15	Closure

Aula Magna, Building A, Faculty of Pharmacy and Food Sciences

Program of the event

II.2 IQTCUB SEMINARS AND CONFERENCES

During 2022 IQTC has organized the following seminars and conferences:

Dr. Birgitte Zeuner (Technical University of Denmark) Denmark
Enzyme technology for oligosaccharide synthesis
February 18th 2022

Dr./Prof. Dimitrios C. Kyritsis (Research and Innovation Center for CO2 and Hydrogen in Khalifa University) United Arab Emirates
Vistas on synthetic fuels – Case studies on light alcohols and ammonia
July 20th 2022

Dr./Prof. Dirk Husmeier (University of Glasgow) United Kingdom
Machine learning to help with inference in the physical sciences: parameter estimation, uncertainty quantification and emulation.
July 11th 2022

Dr./Prof. Peter Kosovan (Charles University, Prague) Czechia
Acid-base equilibria in macromolecular systems - simulations and experiments

September 16th 2022

Dr. Biel Martínez (*Comissariat à l'Énergie Atomique*) France
Quantum computers made of spins: overview of an emerging platform
April 5th 2022

Prof. Carlo Petrongolo (Istituto per i Processi Chimico-Fisici, CNR) Pisa, Italy
Non adiabatic Quantum Theory of Molecules
March 9th 2022

II.3 IQTCUB INVITED RESEARCHERS

During 2022, a total of fourteen researchers have spent some time at the IQTCUB collaborating in different research projects.

1. **Prof. Boris Merinov** (invited visitor, HPC Europa).
   California Institute of Technology (Caltech), USA
   March - April 2022

2. **Elena Zerbato** (visiting Master student).
   University of Trieste, Italy.
   February – May 2022

3. **Prof. Michael A. Robb** (invited visitor)
   Imperial College London, United Kingdom
   September 2022

4. **B. Moses Abraham** (HPC-Europa3 visitor)
   Indian Institute of Technology Kanpur, India
   December 2021-March 2022

5. **Rayene Gara** (invited researcher)
   University of Tunis El Manar, Tunisia
   October-December 2022

6. **Flavio Siro Brigiano** (COST invited visitor)
   Vrije Universiteit Brussel, Belgium
   September 2022

7. **Matteo Lovato** (invited visitor)
   Universita' di Milano Bicocca, Italy
   June-July 2022

8. **Mr. Jhonathan Rosa de Souza** (invited visitor)
   Universidade Federal do ABC, Brazil
   March 2022 – February 2023

9. **Ms. Léxane Fournier** (invited visitor)
   Merck Healthcare KGaA, Germany
   September – December 2022

10. **Dr. Mariano Curti** (invited visitor)
    Institut Català d'Investigació Química, Spain
    February 2022

11. **Prof. Paula Homem de Mello** (invited visitor)
    Universidade Federal do ABC, Brazil
    October 2022

12. **Prof. Petr Jurecka** (invited visitor)
    Palacky University Olomouc, Czech Republic
    September – October 2022

13. **Prof. Marie Zgarbova** (invited visitor)
    Palacky University Olomouc, Czech Republic
    September – October 2022

14. **Prof. Carlo Petrongolo** (HPC-Europa3 invited research)
    Istituto per i Processi Chimico-Fisici, CNR) Pisa, Italy
    February 24th - April 28th ,2022

III. Scientific Activity of IQTCUB Members

III.1 Highlights from most Relevant Results

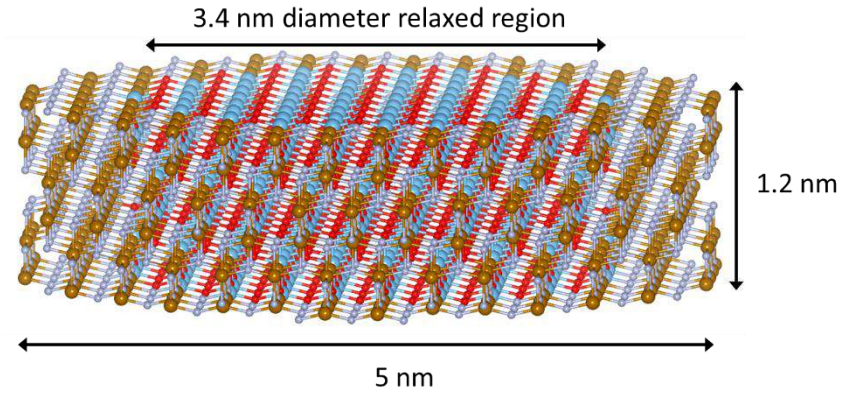
Here some of the most relevant results corresponding to every IQTCUB main research line are presented.

Line 1. Methods, algorithms and computational tools development

Line 2. Computational Materials Science

An Unconstrained Approach to Systematic Structural and Energetic Screening of Materials

G. Di Liberto G, Á. Morales-García, S. T. Bromley ***Nature Communications*** *13 (2022) 6236.*

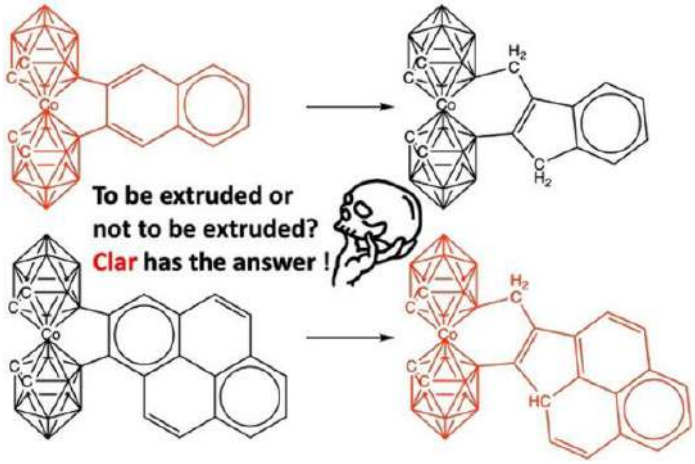


The study introduces a new way to model the stabilities and structures of interfaces using two nanodisks with arbitrary relative twist angles and displacements.

Aromaticity and Extrusion of Benzenoids Linked to [o-COSAN]-. Clar has the Answer

J. Poater, C. Viñas, D. Olid, M. Solà, F. Teixidor

Angew. Chem. Int. Ed., *61* (2022) e202200672.

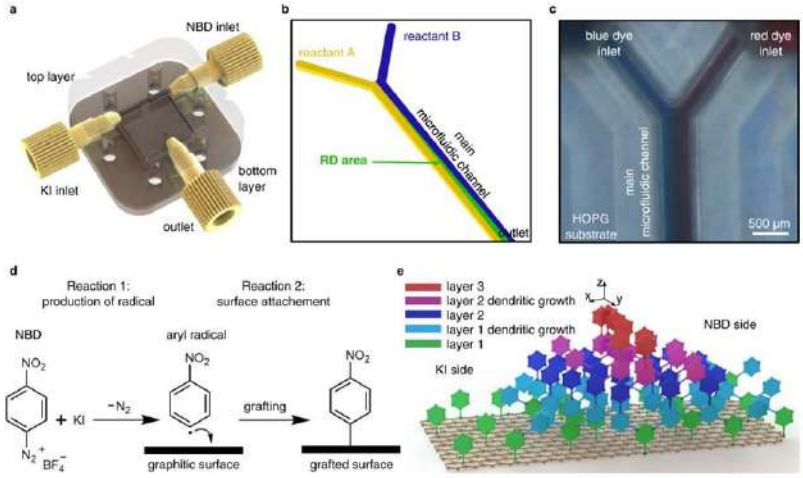


Clar has the answer! Clar's π-sextets justify the reason why the linked system of [o-COSAN]− and benzenoid drives to extrusion in the case of naphthalene or anthracene, but not for benzene, pyrene or perylene.

Covalent transfer of chemical gradients onto a graphenic surface with 2D and 3D control

Yuanzhi Xia, Semih Sevim, João Pedro Vale, Johannes Seibel, David Rodríguez-San-Miguel, Donghoon Kim, Salvador Pané, Tiago Sotto Mayor, Steven De Feyter & Josep Puigmartí-Luis

Nat Commun.,13 (2022) 7006.



a Schematic drawing of the assembled microfluidic device including a Y-shaped microchannel featuring two inlets and one outlet connection ports **b** Illustration of the main microfluidic channel showing the RD area generated inside a continuous-flow microfluidic device. **c** Micrograph of the assembled microfluidic device showing the laminar condition achieved with two food dyes over the HOPG substrate. No leakages or local flow disturbances were observed. Scale bar: 500 µm. **d** Schematic reactions of NBD with KI on a graphitic surface. **e** Illustration showing the dendric growth that can occur with the reactions presented in **d**.

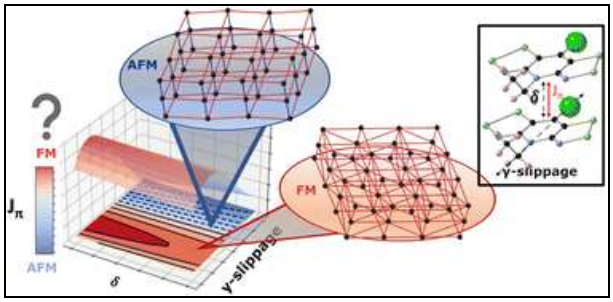
Control over the functionalization of graphenic materials is key to enable their full application in electronic and optical technologies. Covalent functionalization strategies have been proposed as an approach to tailor the interfaces' structure and properties. However, to date, none of the proposed methods allow for a covalent functionalization with control over the grafting density, layer thickness and/or morphology, which are key aspects for fine-tuning the processability and performance of graphenic materials. Here, we show that the no-slip boundary condition at the walls of a continuous flow microfluidic device offers a way to generate controlled chemical gradients onto a graphenic material with 2D and 3D control, a possibility that will allow the sophisticated functionalization of these technologically-relevant materials.

This article was highlighted by the journal.

Magnetic coupling and spin ordering in bisdithiazolyl, thiaselenazolyl, and bisdiselenazolyl molecular materials.

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

Dalton Trans., *51* (2022) 13032.

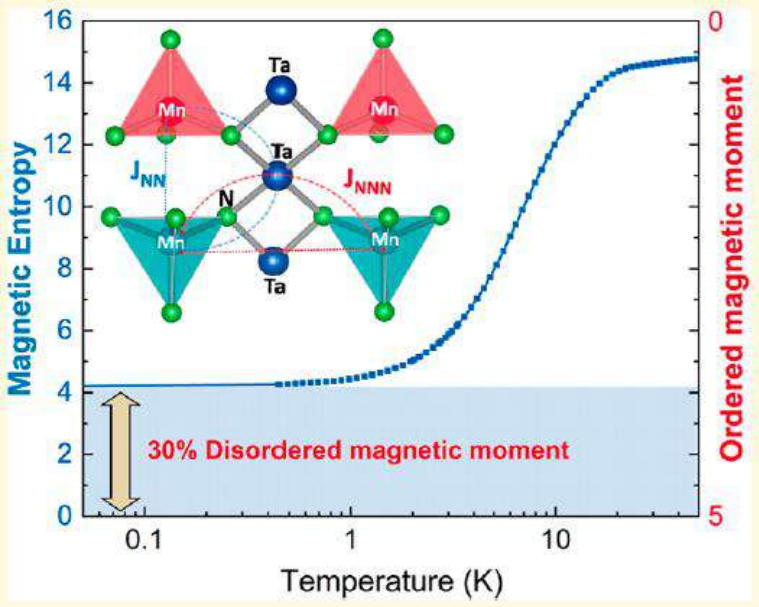


A series of four isostructural bisDTA-derivative multifunctional materials have been computationally investigated triggered by the fact that their magnetic and conducting properties are strongly dependent on different S/Se ratios. X-Ray data at 100 K is only able to rationalise the magnetic response of (S,S) and (Se,S) materials. (S,Se) and (Se,Se) derivatives have been found to be more sensitive to thermal effects, and the expected global FM picture can only be inferred using optimised crystal data at 0 K. The magnetic topologies of both materials show indeed clear differences at 100K/0K, due to the fact that the π-stacking coupling is the most affected by the geometry rearrangements upon temperature cooling. Magneto-structural correlation maps evidence the high sensitivity of the π-stacking couplings to variations in latitudinal slippage and interplanar distances, which can actually be used to tune the very experimental response. Here a variety of useful tools are used to gain insights into the true picture of the overall macroscopic magnetism of the S/Se bisDTA family of multifunctional materials.

$MnTa_2N_4$: A Ternary Nitride Spinel with a Strong Magnetic Frustration.

R.Trócoli, C. Frontera, J. Oró-Solé, C. Ritter, P. Alemany, E. Canadell, M R. Palacín,J. Fontcuberta, A. Fuertes.

Chem. Mater. *34* (2022) 6098-6107.



Magnetic frustration results from competing magnetic interactions leading to unusual ground states such as spin liquids. We report the synthesis of $MnTa_2N_4$ with a normal spinel structure, where the magnetic cations Mn^{2+} occupy exclusively the tetrahedral sites. Although the magnetic interactions are strongly antiferromagnetic ($\theta_{CW} \approx -140$ K), a long-range magnetic order is not established, but a smooth magnetic anomaly is observed at $T^* \approx 5.1$ K, fingerprinting a large magnetic frustration. A short-range helicoidal magnetic order emerges at low temperatures. The ordered moment is ≈70% of the expected magnetic moment of Mn^{2+} ions and a large part of the spin entropy remains at 400 mK, signaling the coexistence of a helicoidal order with spin-liquid-like texture. First-principles calculations unveil an unexpected large direct Mn−Mn exchange interaction that balances the superexchange and accounts for the magnetic frustration.

MXenes à la Carte: Tailoring the Epitaxial Growth Alternating Nitrogen and Transition Metal Layers

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

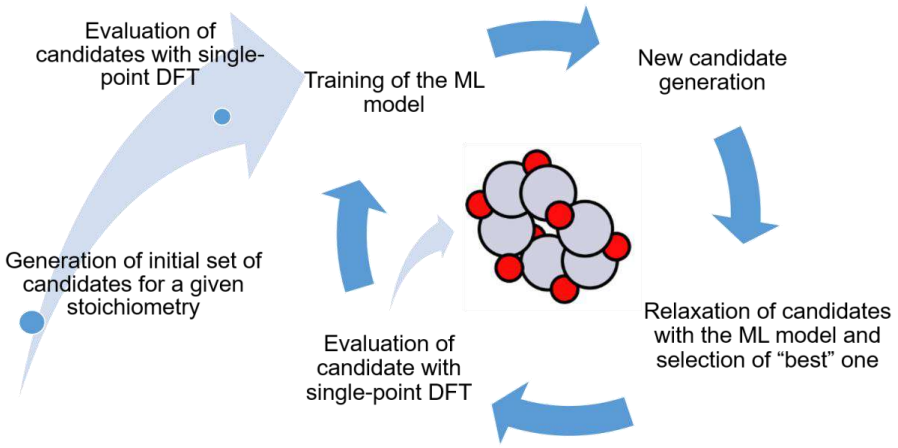
ACS Nano 16 (2022) 12541-12552

A high-throughput analysis based on DFT simulations underscores the viable epitaxial growth of MXenes by alternating nitrogen and metal adlayers. This is supported by an exhaustive analysis of a number of thermodynamic and kinetic thresholds belonging to different critical key steps in the course of the epitaxial growth. The results on 18 pristine N- and C-based MXenes with M2X stoichiometry reveal an easy initial N2 fixation and dissociation, where N2 adsorption is controlled by the MXene surface charge and metal d-band center and its dissociation controlled by the reaction energy change. Furthermore, formation energies indicate the plausible formation of N-terminated M2XN2 MXenes. Moreover, the further covering with metal adlayers is found to be thermodynamically driven and stable, especially when using early transition metal atoms. The present results unfold the possibility of expanding, controlling, and tuning the composition, width, and structure of the MXene family.

Stability of oxidized states of free-standing and ceria-supported PtOx particles.

J.E. Quinlivan Domínguez, K.M. Neyman, A. Bruix.

J. Chem. Phys. *157* (2022) 094709.



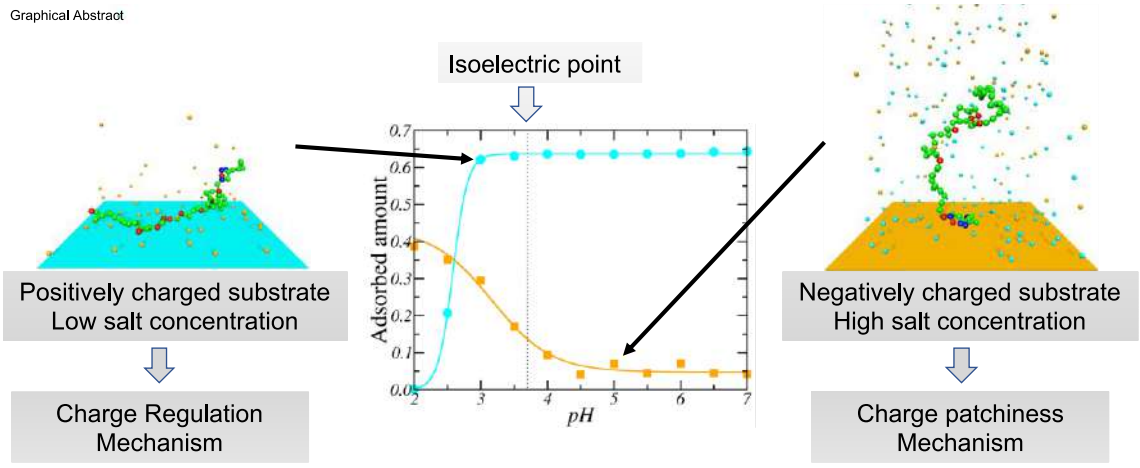
Characterization of Pt/CeO_2 nanomaterials is challenging due to their structural complexity and changes under reaction conditions. This work combined DFT calculations, a machine-learning assisted global optimization method (GOFEE), and ab initio thermodynamics to characterize stable states of ceria-supported Pt_yO_x particles in different environments. The calculated global minima structures for different stoichiometries are used to assess the effects of temperature, O_2 pressure, and support interactions on the phase diagrams, oxidation states, and geometries of the Pt_yO_x particles. Thus identified favoured structural motifs and O:Pt ratios revealed that oxidized free-standing and ceria-supported platinum particles are more stable than reduced ones under a wide range of conditions. Therefore, the studies rationalizing activity of ceria-supported Pt clusters must consider oxidized states and the previous understanding of such materials obtained only with fully reduced Pt clusters may be incomplete.

LINE 3. COMPUTATIONAL BIOCHEMISTRY AND SOFT MATTER

Adsorption of flexible proteins in the 'wrong side' of the isoelectric point: Casein macropeptide as a model system.

Blanco, P.M.; Achetoni, M.M.; Garcés, J.L.; Madurga, S.; Mas, F.; Baieli, M.F.; Narambuena, C.F.

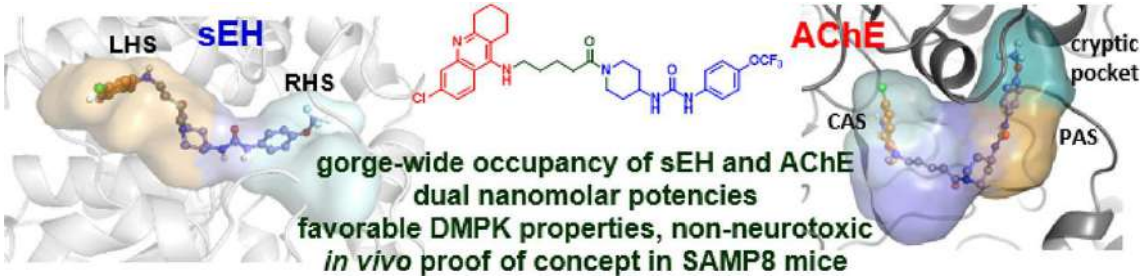
Cooloids Surface B. Biointerfaces., *217* (2022) 112617.



We analyze the conditions for the adsorption of a flexible peptide onto a charged substrate in the "wrong side" of the isoelectric point (WSIP), *i.e.*, when surface and peptide charges have the same sign. As a model system, we focus on the casein macropeptide (CMP), both in the aglycosylated (aCMP) and fully glycosydated (gCMP) forms. We model the substrate as a uniformly charged plane while CMP is treated as a bead-and-spring model including electrostatic interactions, excluded volume effects and acid/base equilibria. Adsorption coverage, aminoacid charges and concentration profiles are computed by means of Monte Carlo simulations at fixed pH and salt concentration. We conclude that CMP can be adsorbed in the WSIP to both positively and negatively charged surfaces, although for different reasons. For negatively charged surfaces, WSIP adsorption is due to the patchy distribution of charges: the peptide is attached to the surface by the positively charged end of the chain, while the repulsion of the surface for the negatively charged tail is screened by the small ions of the added salt. This effect increases with salt concentration. Conversely, a positively charged substrate induces strong charge regulation of the peptide: the acidic groups are deprotonated, and the peptide becomes negatively charged. This effect is stronger at low salt concentrations and it is more intense for gCMP than for aCMP, due to the presence of the additional sialic groups in gCMP.

Discovery and In Vivo Proof of Concept of a Highly Potent Dual Inhibitor of Soluble Epoxide Hydrolase and Acetylcholinesterase for the Treatment of Alzheimer's Disease

Codony, B. Pont, C. Griñán-Ferré, C. Di Pede-Mattatelli, A. Calvó-Tusell, C. Feixas, F. Osuna, S. Jarné-Ferrer, J. Naldi, M. Bartolini, M. Loza, M.I. Brea, J. Pérez, B. Bartra, C. Sanfeliu, C. Juárez-Jiménez, J. Morisseau, C. Hammock, B.D. Pallàs, M. Vázquez*, M. and Muñoz-Torrero, D. **J. Med. Chem.**, *65,6,* (2022) 4909-4925.

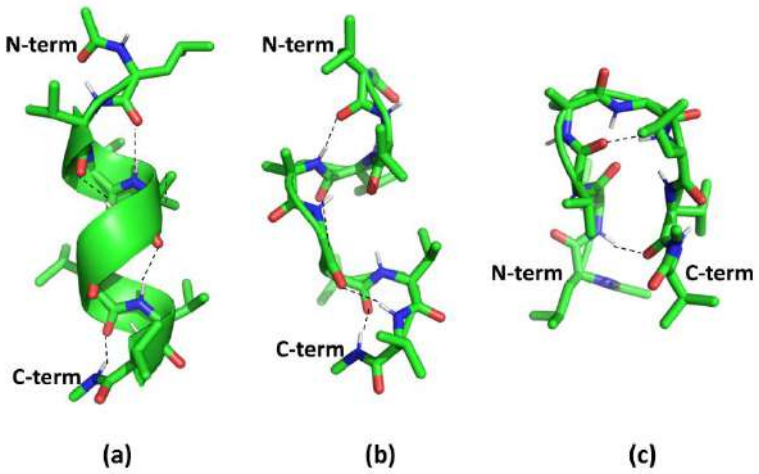


With innumerable clinical failures of target-specific drug candidates for multifactorial diseases, such as Alzheimer's disease (AD), which remains inefficiently treated, the advent of multitarget drug discovery has brought a new breath of hope. Here, we disclose a class of 6-chlorotacrine (huprine)–TPPU hybrids as dual inhibitors of the enzymes soluble epoxide hydrolase (sEH) and acetylcholinesterase (AChE), a multitarget profile to provide cumulative effects against neuroinflammation and memory impairment. Computational studies confirmed the gorge-wide occupancy of both enzymes, from the main site to a secondary site, including a so far non-described AChE cryptic pocket. The lead compound displayed in vitro dual nanomolar potencies, adequate brain permeability, aqueous solubility, human microsomal stability, lack of neurotoxicity, and it rescued memory, synaptic plasticity, and neuroinflammation in an AD mouse model, after low dose chronic oral administration.

Effects of solvents on the conformational profile of Balaram's peptide: a computational study.

Patricia Gomez-Gutierrez; Jaime Rubio-Martinez; Juan J. Perez

Phys. Chem. Chem. Phys., **24** (2022) 27879-27892

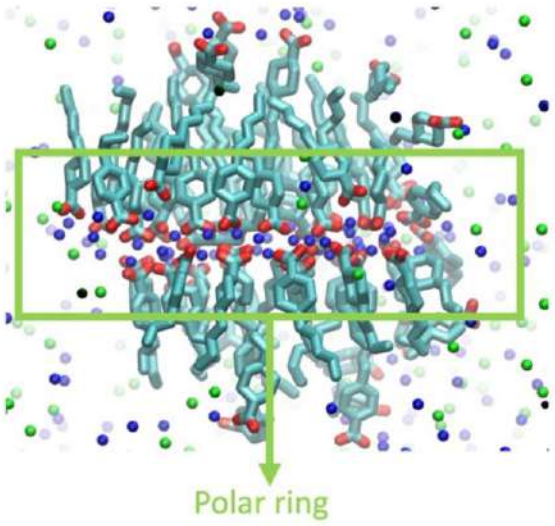


This work reports the results of a computational study aimed at characterizing the conformational profile of the Balaram's peptide in different solvents, including chloroform, dimethyl sulfoxide, methanol and water. For this purpose, 10 μs molecular dynamics trajectories were computed in explicit solvent for each system, starting from an extended conformation. The results of the present study confirm previous NMR and CD findings.

Naphthenic Acids Aggregation: The Role of Salinity.

R.D. Cunha, L.J. Ferreira, E. Orestes, M.D. Coutinho-Neto, J.M. de Almeida, R.M. Carvalho, C.D. Maciel, C. Curutchet, P. Homem-de-Mello.

Computation, *10* (2022) 170.

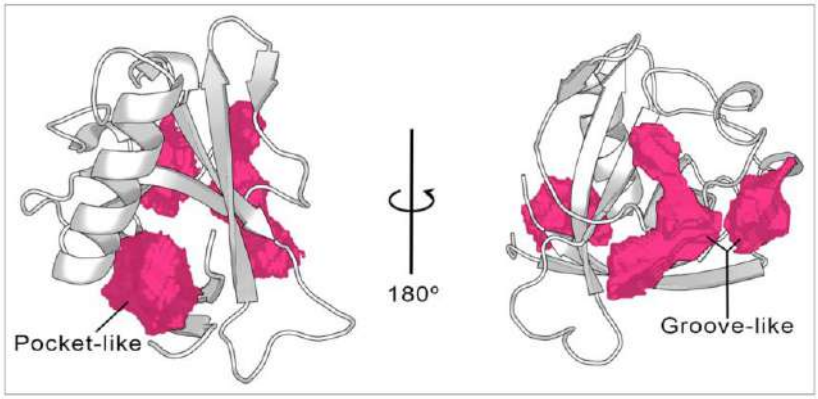


Naphthenic Acids (NA) are important oil extraction subproducts. These chemical species are one of the leading causes of marine pollution and duct corrosion. For this reason, understanding the behaviour of NAs in different saline conditions is one of the challenges in the oil industry. In this work, we simulated several NA species and their mixtures, employing quantum chemical continuum solvation models and explicit-solvent classical molecular dynamics simulations. Our results indicated that the longer chain acids are more hydrophobic and lead to higher order aggregates. We also found that larger aggregates are stable at higher salinities, which can explain the observed low-salinity-enhanced oil recovery. Interestingly, our simulations showed that stabilization of the aggregates induced by the salinity involves a direct interplay of Na^+ cations with the carboxylic groups of the NAs inside the aggregates.

Revealing druggable cryptic pockets in the Nsp1 of SARS-CoV-2 and other β-coronaviruses by simulations and crystallography.

A. Borsatto, O. Akkad, I. Galdadas, S. Ma, S. Damfo, S. Haider, F. Kozielski, C. Estarellas, FL. Gervasio

Elife, *11* (2022) 81167.



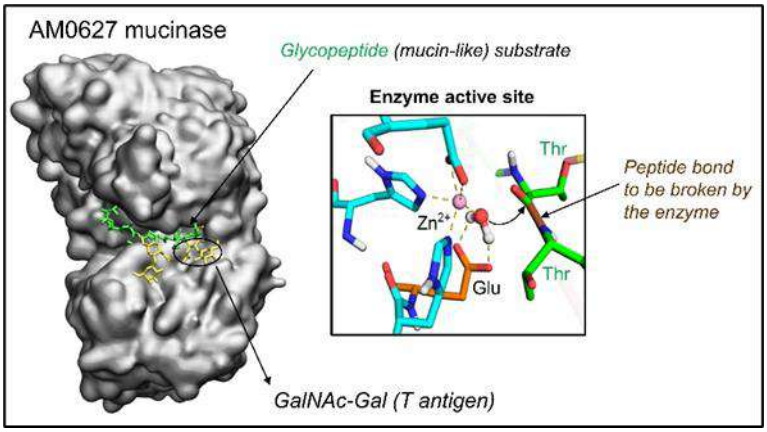
Non-structural protein 1 (Nsp1) is a main pathogenicity factor of α- and β-coronaviruses. Nsp1 of SARS-CoV-2 suppresses the host gene expression by sterically blocking 40S host ribosomal subunits and promoting host mRNA degradation. This mechanism leads to the downregulation of the innate immune response in host cells, ultimately mediating the observed immune evasion capabilities of SARS-CoV-2. Here, by combining molecular dynamics simulations, fragment screening and crystallography, we reveal druggable pockets in Nsp1. Structural and computational solvent mapping analyses indicate the partial crypticity of these newly discovered and druggable binding sites. The results of fragment-based screening via X-ray crystallography confirm the druggability of the major pocket of Nsp1. Finally, we show how the

targeting of this pocket could disrupt the Nsp1-mRNA complex and open a novel avenue to design new inhibitors for other Nsp1s present in homologous β-coronaviruses.

Structural and mechanistic insights into the cleavage of clustered O-glycan patches-containing glycoproteins by mucinases of the human gut.

V. Taleb, Q. Liao, Y. Narimatsu, A. García-García, I. Compañón, R. J. Borges, A. M. González-Ramírez, F. Corzana, H. Clausen, C. Rovira, R. Hurtado-Guerrero.

Nat. Commun. 13 (2022) 4324



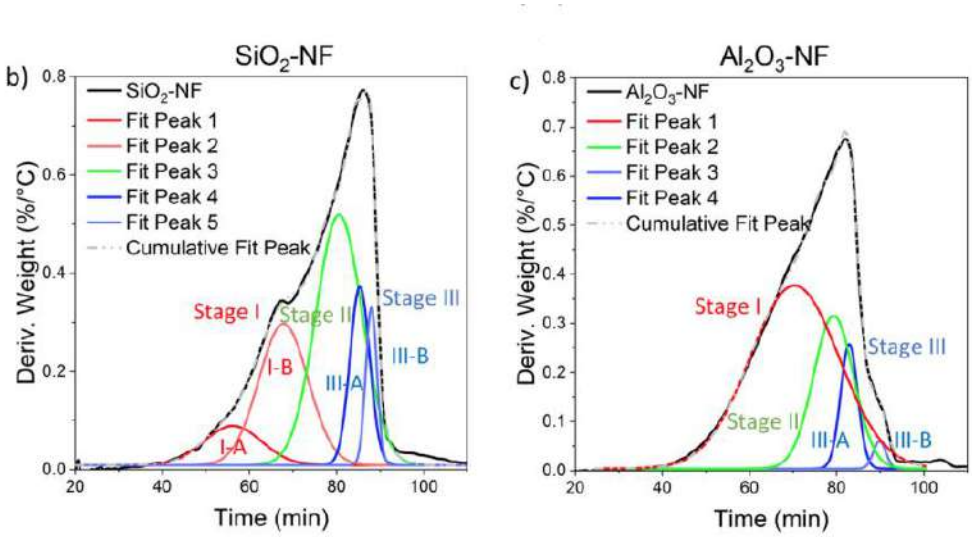
Mucins are a type of highly glycosylated proteins present in the mucus layers of most organisms (e.g. the intestinal mucus). They contribute to protect us from external microorganisms, avoiding that they reach the epithelial cells. Mucins are degraded by specific enzymes, named mucinases, which contribute to mucus regeneration. Recently, we have uncovered the mechanism of action of a mucinase secreted by the bacteria *Akkermansia muciniphila*, by means of a multidisciplinary work involving protein structure determination, synthetic biology and molecular simulations. Our results show that the enzyme is able to recognize two contiguous aminoacids (residues) that are glycosylated, with preference for each of them containing two sugars of *N*-acetylgalactosamine and galactose (GalNAc-Gal, named T antigen). Once the enzyme binds to these specific glycosylation sites, it cleaves the peptide bond between the two glycosylated residues via a concerted mechanism relying on a nucleophilic water molecule. Our work illustrates how mucinases, through tremendous flexibility, adapt to the diversity in distribution and patterns of *O*-glycans on mucins.

LINE 4. REACTIVITY AND REACTIONS DYNAMICS

Effect of Nanoparticles on the Thermal Stability and Reaction Kinetics in Ionic Nanofluids.

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

Nanomaterials, *12* (2022) 1777.

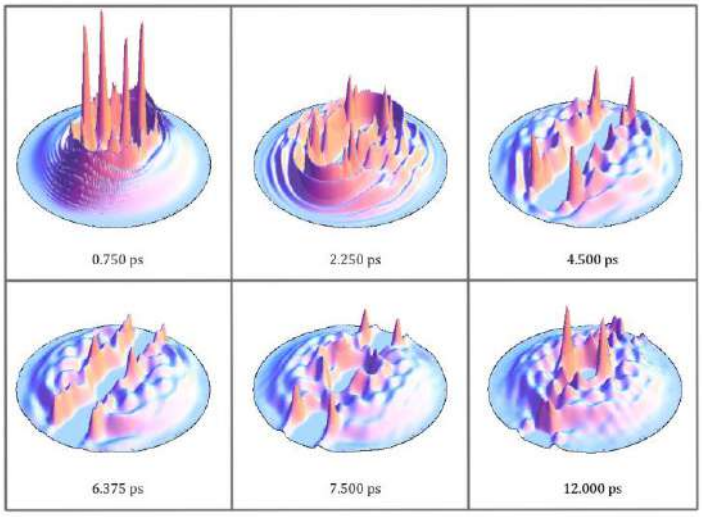


Nowadays, the incorporation of nanoparticles into thermal fluids has become one of the most suitable strategies for developing high-performance fluids. An unconventional improvement of thermo–physical properties was observed with the addition of 1% wt. of nanoparticles in different types of fluids, such as molten salts, allowing for the design of more thermally efficient systems using nanofluids. Despite this, there is a lack of knowledge about the effect that nanoparticles produce on the thermal stability and the decomposition kinetics of the base fluid. The present study performs IR- and UV-vis spectroscopy along with thermogravimetric analysis (TGA) of pure nitrate and nitrate based nanofluids with the presence of SiO2 and Al2O3 nanoparticles (1% wt.). The results obtained support that nanoparticles accelerate the nitrate to nitrite decomposition at temperatures below 500 °C (up to 4%), thus confirming the catalytic role of nanoparticles in nanofluids.

Quantum dynamics of the Br_2 (B-excited state) photodissociation in superfluid helium nanodroplets: importance of the recombination process

A. Vilà, M. González. Phys. Chem. Chem. Phys.,

Phys. Chem. Chem. Phys., *24* (2022) 24353.



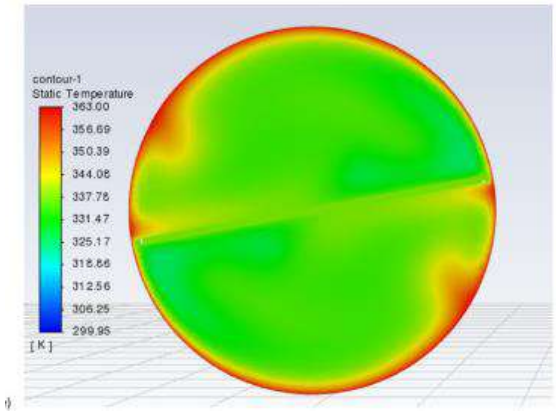
The Br_2 photodissociation dynamics (B←X electronic transition) of Br_2(v=0,X)@(^{4}He)$_N$ superfluid doped helium nanodroplets (T=0.37 K) at zero angular momentum (N: 100–1000), was studied using a quantum mechanical (QM) approach proposed by us. This is the second QM dynamics study available on the photodissociation of molecules in (^{4}He)$_N$ and while some properties are qualitatively similar to those previously reported by us for Cl_2 (e.g., the oscillating Br final velocity distribution arising from quantum interferences appearing shortly after the excitation), large differences are evident in other properties: photodissociation mechanism (much more complex for Br_2 and leading to the fragmentation of the initial wave packet), dissociation probability and time scale of the process. The results were satisfactorily interpreted from the significantly lower excitation energy achieved by the Br_2(B←X) transition and the higher reduced mass of Br_2 in comparison to Cl_2.

LINE 5. COMPUTATIONAL FLUID DYNAMICS

Heat transfer in pipes with twisted tapes: CFD simulations and validation

Cabello, R., Plesu Popescu, A.E., Bonet-Ruiz, J., Curcó Cantarell, D., Llorens, J.

Computers and Chemical Engineering, *166* (2022) 107971.



Inserts are placed inside heat exchangers to promote turbulence and maximize the heat transferred. Twisted tapes enhance heat transfer with minimal pressure drop increase for double pipe heat exchangers. Their design typically relied on experimental correlations, but nowadays CFD software is gaining interest. The choice of the turbulent model is of paramount importance and not addressed in the literature. Results provide clues for choosing a suitable turbulent model and are useful to minimize the error provided by the models.

III.2 PUBLICATION LIST

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(1) Aledavood, E.; Selmi, B.; Estarellas, C.; Masetti, M.; Luque, F. J., From Acid Activation Mechanisms of Proton Conduction to Design of Inhibitors of the M2 Proton Channel of Influenza A Virus. ***Frontiers in Molecular Biosciences*** *8*, (2022), 796229 10.3389/fmolb.2021.796229.

(2) Allès, M.; Remesal, E. R.; Illas, F.; Morales-García, Á., Structural and Electronic Properties of Metal/Oxide Nanostructures from First-Principles: Ru13 Supported on (TiO2)84 as a Case Study. ***Advanced Theory and Simulations***, (2022), 10.1002/adts.202200670.

(3) Almeida, M. O.; Kolb, M. J.; Lanza, M. R. V.; Illas, F.; Calle-Vallejo, F., Gas-Phase Errors Affect DFT-Based Electrocatalysis Models of Oxygen Reduction to Hydrogen Peroxide. ***ChemElectroChem*** *9*, (2022), e202200210 10.1002/celc.202200210.

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(8) Arulmozhi, N.; Hanselman, S.; Tudor, V.; Chen, X.; van Velden, D.; Schneider, G. F.; Calle-Vallejo, F.; Koper, M. T. M., Energetics and Kinetics of Hydrogen Electrosorption on a Graphene-Covered Pt(111) Electrode. ***Journal of the American Chemical Society***, (2022), 10.1021/jacsau.2c00648.

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(10) Bagus, P. S.; Sousa, C.; Illas, F., XPS binding energy shifts as a function of bond distances: A case study of CO. ***Journal of Physics Condensed Matter*** *34*, (2022), 154004 10.1088/1361-648X/ac4dc0.

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(13) Belle, R.; Kamps, J. J. A. G.; Poater, J.; Kumar, K.; Pieters, B. J. G. E.; Salah, E.; Claridge, T. D. W.; Paton, R. S.; Bickelhaupt, F. M.; Kawamura, A.; Schofield, C. J.; Mecinović, J., Reading and erasing of the phosphonium analogue of trimethyllysine by epigenetic proteins. ***Communications Chemistry*** *5*, (2022), 27 10.1038/s42004-022-00640-4.

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(17) Bofill, J. M.; Quapp, W.; Albareda, G.; Moreira, I. D. P. R.; Ribas-Ariño, J., Controlling Chemical Reactivity with Optimally Oriented Electric Fields: A Generalization of the Newton Trajectory Method. ***Journal of Chemical Theory and Computation*** *18*, (2022), 935-952 10.1021/acs.jctc.1c00943.

(18) Borsatto, A.; Akkad, O.; Galdadas, I.; Ma, S.; Damfo, S.; Haider, S.; Kozielski, F.; Estarellas, C.; Gervasio, F. L., Revealing druggable cryptic pockets in the Nsp1 of SARS-CoV-2 and other β-coronaviruses by simulations and crystallography. ***eLife*** *11*, (2022), e81167 10.7554/eLife.81167.

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BOOK CHAPTERS AND PROCEEDINGS

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

III.3 OTHER ACTIVITIES

PHD THESES 2022

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

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

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

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

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

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

Computational modelling of magnetic and conducting properties of multifunctional molecular materials.
Cristina Roncero Barrero
Facultat de Química, Universitat de Barcelona.
Química Teòrica i Modelització Computacional
Mercè Deumal i Solé , Ibério de P. Ribeiro Moreira
September 2022

Computational Analyses of CO_2 Electroreduction and C Interactions with Transition Metals
Oriol Piqué Caufapé
Facultat de Química, Universitat de Barcelona.
Theoretical and Computational Chemistry
Francesc Viñes & Federico Calle-Vallejo
May 2022

Nitrate salt-based nanofluids for thermal energy storage.
Adela Svobodova Sedlackova
Facultat de Química, Universitat de Barcelona.
Enginyeria i Ciències Aplicades
Supervisors: Ana Ines Fernández i Pablo Gamallo
July 2022

MASTER THESES 2022

Effect of oxygen adsorption on optical properties of Ag nanoparticles.
Elena Zerbato
Dipartimento di Scienze Chimiche e Farmaceutiche, Università di Trieste (Italy)
MSc program: Master in Chemistry
Supervisor/s: Mauro Stener, Konstantin Neyman
July 2022

Improvement of the fragrance process design based on the experimental raw material data
María Montañés Puig
Facultat de Química, Universitat de Barcelona.
Master on Chemical Engineering
Supervisor/s: Jordi Bonet Ruiz; Alexandra Elena Plesu Popescu
February 2022.

Contribution to the study of heat integration of pressure swing distillation
Eva Gutiérrez Campos
Facultat de Química, Universitat de Barcelona.
Master on Chemical Engineering
Supervisor/s: Jordi Bonet Ruiz; Víctor Manso
February 2022.

Methanol synthesis by CO2 hydrogenation using reactive distillation
Eric Meco Morales
Facultat de Química, Universitat de Barcelona.
Master on Chemical Engineering
Supervisor/s: Jordi Bonet Ruiz; Alexandra Elena Plesu Popescu
February 2022.

Improvement of the p-xylene and benzene production process through the disproportionation of the toluene
Xavier Valldepérez González
Facultat de Química, Universitat de Barcelona.
Master on Chemical Engineering
Supervisor/s: Jordi Bonet Ruiz; Alexandra Elena Plesu Popescu
June 2022.

Study and control design of an industrial clinker precalciner
Manuel Torcida Arévalo
Facultat de Química, Universitat de Barcelona.
Master on Chemical Engineering
Supervisor/s: Jordi Bonet Ruiz; Alexandra Elena Plesu Popescu
June 2022.

Daniel Conde Torres
Facultat de Química, Universitat de Barcelona.
Màster en Modelització Computacional Atomística i Multiescala en Física, Química i Bioquímica
R. García Fandiño & C. Rovira
July 2022

Use of AlphaFold and other computational methods in glycosyltransferase research
Òscal Vidal Gironès
Facultat de Química, Universitat de Barcelona.
Màster de Química Orgànica
C. Rovira & Q. Liao
July 2022

Confined synthesis of functional matter and its effects on morphogenesis.
Gemma Llauradó Capdevila
Facultat de Química, Universitat de Barcelona.
Màster de Química de Materials Aplicada
Josep Puigmartí Luis
July 2022.

Crystallization of peptide-based MOFs gels controlling the diffusion of solvents across PDMS membranes.
Martí Sanz Mir
Facultat de Química, Universitat de Barcelona.
Màster de Química de Materials Aplicada
Josep Puigmartí Luis
July 2022.

On the use of Markov State Models in the fragment dissolved Molecular Dynamics method.
Maria Nuria Peralta Moreno
Facultat de Química, UB; International Centre for Theoretical Physics.
Theoretical Chemistry and Computational Modelling
Jaime Rubio Martínez , Alejandro Rodríguez García
July 2022.

Search for glutaminase inhibitors by molecular modeling.
Albert Álvarez Muñoz
Facultat de Química, UB.
Modelització Computacional Atomística i Multiescala en Física, Química i Bioquímica
Jaime Rubio Martínez
July 2022.

Uncover the biological activity of dark chemical matter as SARS-CoV-2 inhibitors.
Yago Mena Barrientos
Facultat de Química, UB.
Applied Materials Chemistry
Jaime Rubio Martínez
July 2022

Jorge Duro Sánchez
Facultat de Farmàcia i Ciències de L'Alimentació , Universitat de Barcelona.
Biotecnologia
Jordi Juárez-Jiménez
Julio 2022

Structural basis of the selective direct activation mechanism of AMPK: Isoform dependent complexes.
Katerina Barmpidi
UB - UPC
Atomistic and Multiscale Computational Modelling in Physics, Chemistry and Biochemistry
Supervisor/s: C. Estarellas
July 2022.

Accurate prediction of the nature of the electronic ground state of MXenes
Néstor Mauricio García-Romeral González
Facultat de Química, Universitat de Barcelona.
Erasmus Mundus Theoretical Chemistry and Computational Modelling
Ángel Morales García & Francesc Illas Riera
July 2022.

CO_2 methanation on MXenes: Assessment by DFT screening and kinetic Monte Carlo
Daniel Dolz García
Facultat de Química, Universitat de Barcelona.
Erasmus Mundus Theoretical Chemistry and Computational Modelling
Ángel Morales García & Francesc Viñes Solana
June 2022.

Thermodynamic, kinetic, and dynamic aspects of the separation of CO_2 from light fuels using nano-engineered grazynes
Adrià Calzada Escrig
Facultat de Química, Universitat de Barcelona.
Atomistic and Multiscale Computational Modelling in Physics, Chemistry and Biochemistry
Francesc Viñes Solana & Pablo Gamallo Belmonte
July 2022.

Systematic study, from first principles calculations, of adsorption and dissociation of probe CO molecule on low Miller indices transition metal surfaces.
David Vázquez Parga
Facultat de Química, Universitat de Barcelona.
Erasmus Mundus Theoretical Chemistry and Computational Modelling
Francesc Viñes Solana
June 2022.

Dynamics of the reverse water gas shift reaction on Mo_2C MXene
Raúl De Armas Rodríguez
Facultat de Química, Universitat de Barcelona.
Atomistic and Multiscale Computational Modelling in Physics, Chemistry and Biochemistry
Francesc Viñes Solana
September 2022.

Benchmark: quantum-augmented excited state force-fields for protein fluorescence
Mateus Zanotto
Facultat de Farmàcia i Ciències de l'Alimentació, Universitat de Barcelona.
Erasmus Mundus Master in Theoretical Chemistry and Computational Modelling
Prof. Carles E. Curutchet (University of Barcelona) & Prof. Shirin Faraji and Dr. Maximilian Menger (University of Groningen)
June 2022.

Sampling of porous materials for post-combustion flue gas by using Grand Canonical Monte Carlo and Computational Fluid Dynamics Simulations.
Jorge Cardenas Gamboa
Facultat de Química, Universitat de Barcelona.
Erasmus Mundus on Theoretical Chemistry and Computational Modelling
Supervisors: Pablo Gamallo.
July 2022.

Improvement of the p-xylene and benzene production process through the disproportionation of the toluene.
Xavier Valldepérez González
Facultat de Química, Universitat de Barcelona.
Enginyeria Química
Supervisors: Alexandra Plesu, Jordi Bonet
July 2022.

Design of an agitated tank for heating glucose syrup
Erika Fernandez Pizarro
Facultat de Química, Universitat de Barcelona.
Supervisors: Ruben Cabello, Alexandra Plesu
July 2022.

Study and control design of an industrial clinker precalciner
Manuel Fidel Torcida Arévalo
Supervisors: Jordi Bonet, David Curcó
Facultat de Química, Universitat de Barcelona.
TFM a empresa: Ciments Molins (tutora: Eva Sebastià)
July 2022.

Modelling interatomic interactions in titanium carbide by machine learning
Jorge Refugio Fabila Fabian
Facultat de Química, Universitat de Barcelona.
Máster de Química Teórica y Modelización Computacional
Stefan T. Bromley & Julien Lam
June 2022

Predicting possible molecular structures for hydroxylated silica nanoclusters from infrared spectra using machine learning methods
Andreu A. de Donato
Facultat de Química, Universitat de Barcelona.
Máster de Química Teórica y Modelización Computacional
Stefan T. Bromley & Jordi Ribas
July 2022

Constant-pH simulations of a coarse-grained model of flexible linear polyelectrolytes.
David Alejandro Naranjo Tovar
Facultat de Química, Universitat de Barcelona.
Modelització Computacional Atomística i Multiescala en Física, Química i Bioquímica
Dr. Sergio Madurga and Dr. Francesc Mas
July 2022

Estimating the electronic stopping power of materials through non-adiabatic molecular dynamics and machine learning techniques.
Ferran Jiménez Cuélliga
Facultat de Química, Universitat de Barcelona.
Atomistic and Multiscale Computational Modelling in Physics, Chemistry and Biochemistry
Pere Alemany.
July 2022.

BACHELOR THESES 2022

Neuraminidase superfamily compendium
Alba Recio Sierra
Facultat de Química, Universitat de Barcelona
Grau de Química
C. Rovira.
January 2022

ORGANIZATION OF CONGRESSES 2022

Cluster-Surface Interaction workshop (CSI2022), April 1-4, 2022
Santa Margherita Ligure (Italy)
Congress Organization
Charing a session on April 3, 2022

School "Hybrid Quantym Mechanics / Molecular Mechanics (QM/MM) Approaches to Biochemistry and Beyond"
Centre Européen de Calcul Atomique et Moléculaire (CECAM), EPFL Lausanne (Switzerland)
May 2022
Organizers: M. Boero, A. Seitsonen, P. Campomanes, C. Rovira

Symposium "Molecules, Macromolecules and Biomolecules" within the Psi-K 2022 conference
Centre Européen de Calcul Atomique et Moléculaire (CECAM), EPFL Lausanne (Switzerland)
August 2022
Organizers: C. Molteni, C. Rovira

Cicle de conferències 'Ask along the expert talks'
Aula Casassas, Universitat de Barcelona
Programa de Doctorat en Química Teòrica i Modelització Computacional
Chairwoman: M.Deumal com a coordinadora del Programa de Doctorat

IQTC Meeting 2022
Faculty of Chemistry, Barcelona (Spain)
Celebration date (format: 19-20/07/2022)
Congress Organization
Chairman or Organizers: E. Ruiz, C. Curutchet, J. Juarez-Jimenez, C. Estarellas

Simposio "Carburos y nitruros nanolaminados de metales de transición (MAX y MAB) y sus correspondientes materiales 2D (MXenes and MBenes)"
Instituto de Cerámica y Vidrio, Madrid (Spain)
LVIII Congreso Nacional de la Sociedad Española de Cristal y Vidrio
Chairman: Ángel Morales García

NANOWS 2022 – Achievements and challenges of multiscale modelling of nanocrystals for eficient water splitting
University of Aveiro, Aveiro (Portugal)
Chairman: Francesc Viñes

Allosterism & Drug Discovery Conference
University of Barcelona, Barcelona (Spain)
Congress organization
Chairman or Organizers: Carles E. Curutchet and Xavier Barril

New Trends in Computational Chemistry 2022: Introducing the Quantum Revolution in Chemistry High-Performance Computing
University of Barcelona, Barcelona (Spain)
Congress organization
Chairman or Organizers: Eliseo Ruiz, Francesc Viñes, Jesús Jover and Carles E. Curutchet

CECAM School con Kinetics and Dynamics of Chemical Reactions
9-13/05/2022 - Zaragoza (Spain)
Congress organization
Pablo Gamallo

9th European Conference on Boron Chemistry
UAB, July 2022, Barcelona (Spain)
Scientific Organizing commitee: J. Poater

1st Symposium of the Working Group 3 "Confined Metal and Metal-Oxide Nanoparticles and Clusters Down to the Subnanometer Scale" of the COST Action 21101
On-line
19/12/2022
DFT prediction of unexpectedly easy oxidation of small Pt clústers (short talk)
K. Neyman
Development of grand canonical global optimization methods for the characterization of materials under reaction conditions (short talk)
A. Bruix

International Workshop on Non-Equilibrium and Environment Effects on Nanoalloys,
Paris (France)
7-9/12/2022.
Modelling chemical ordering in bimetallic nanoparticles: Effects of reactive environament (talk)
K. Neyman
The NanoParticleLibrary: a python package for computational studies of Nanoalloys (talk)
A. Bruix

PRACE Catalysis for Europe's Green Transition: Workshop on advancing industrial catalysis by synergy of experiments and supercomputing simulations
Sofia (Bulgaria)
21-25/11/2022
Introduction to machine learning for catalysis (invited online lecture)
A. Bruix

4th International Conference on Materials: Advanced and Emerging Materials
Barcelona (Spain)
19-21/10/2022
In-silico designing bimetallic nanoparticles (invited lecture)
K. Neyman

NanoGe International Conference on Frontiers in Electrocatalytic Transformations (INTERECT22)
Valencia (Spain)
21-22/10/2022
Modeling the Structural and Environmental Complexity in Working Catalysts
A. Bruix

VII International School-Conference "Catalysis: from Science to Industry"
Tomsk (Russia)
11-15/10/2022
Computational modelling of bimetallic nanoparticles in catalysis (plenary lecture on-line)
K. Neyman

Faraday discussion "Nanoalloys: recebt developments and future perspectives"
London (UK)
21-23/09/2022
The NanoParticleLibrary: a python package for computational studies of nanoalloys (short talk and poster)
R. Farris

3rd Summer School "Colloid and interface research & innovations", project EXTREME
Varna (Bulgaria)
9-11/07/2022
Quantifying interface effects in catalysis combining computer modelling and experiment (invited lecture on-line)
K. Neyman

ZCAM-ASEVA Workshop Metal-Oxide Ultrathin Films and Nanostructures
Zaragoza (Spain)
4-8/07/2022
Quantifying metal/metal-oxide interface effects in catalytic nanomaterials (keynote lecture)
K. Neyman
4-8/07/2022
Systematic approach to electron transfer for ceria supported metal particles
P. Castro

EMMC-eSSENCE Intern. meeting on "Multiscale modelling of materials and molecules"
Uppsala (Sweden)
1-3/06/2022
Ordering in bimetallic nanoparticles: Effects of environment (invited lecture)
K. Neyman

Department of Physical Electronics, Tel Aviv University
Tel Aviv (Israel)
09/05/2022
Metal/metal-oxide interface effects in catalytic nanomaterials: Density functional modelling versus experiment (invited lecture)
K. Neyman

Department of Materials Science and Engineering, TECHNION - Israel Inst. of Technology
Haifa (Israel)
08/05/2022
Quantifying metal/metal-oxide interface effects in catalytic nanomaterials: Density functional modelling versus experiment (invited lecture)
K. Neyman

Spring School on Nanoalloys (Nanoalloys International Research Network)
Cargèse, Corsica (France)
24-30/04/2022
Influence of non-local properties on the adsorption energies on metal nanoparticles (poster)
R. Farris

Cluster-Surface Interaction workshop (CSI2022)
Santa Margherita Ligure (Italy)
1-4/04/2022
DFT modelling of oxide-supported metal clusters and nanoparticles relevant to catalysis (invited lecture)
K. Neyman

Kings College London. Biological Physics Across Scales (BiPAS) seminar series
New catalytic mechanisms in carbohydrate-active enzymes (CAZymes) unveiled by computer simulation
C. Rovira
April 2022

Mixed-gen Season 2 – Session 6 Simulating biological Systems (CECAM)
Online Meeting hosted by CECAM-HQ, Lausanne (Switzerland)
31/March/2022
Modeling Bifidobacterium bifidum*'s lacto-N -biosidase by means of Molecular Dynamics* (poster)
I. Cuxart, J. Coines, O. Esquivias, M. Faijes, A. Planas, X. Biarnés, C. Rovira
Asparagine Tautomerization in Glycosyltransferase Catalysis. The Molecular Mechanism of Protein O-Fucosyltransferase 1 (talk & poster)
B. Piniello, E. Lira-Navarrete, H. Takeuchi, M. Takeuchi, R. S. Haltiwanger, R. Hurtado-Guerrero, C. Rovira

1st Network Meeting on Glycan Structural Biology, Analytics & Computational Studies
Naples (Italy)
4/April/2022 – 6/April/2022
Computer simulation of unusual reaction mechanisms in glycosidases (talk)
C. Rovira

Hybrid Quantum Mechanics/Molecular Mechanics (QM/MM) Approaches to Biochemistry and Beyond (CECAM)
CECAM-HQ-EPFL, Lausanne (Switzerland)
16/May/2022 – 20/May/2022
Modeling Bifidobacterium bifidum*'s lacto-N -biosidase by means of Molecular Dynamics* (flash presentation & poster)
I. Cuxart, J. Coines, O. Esquivias, M. Faijes, A. Planas, X. Biarnés, C. Rovira

VI Conference of Predoctoral Researchers de l'Escola de Doctorat de la UdG
Facultat de Ciències, Universitat de Girona, Girona (Spain)
30/May/2022
Simulation of enzyme reactions in glycoside hydrolases (talk)
I. Cuxart, J. Coines, O. Esquivias, M. Faijes, A. Planas, X. Biarnés, C. Rovira

Girona Seminar 2022
Auditori de la Mercè, Girona (Spain)
31/May/2022 – 3/June/2022
Computer simulation of new reaction mechanisms in glycosidases (talk)
C. Rovira

IRP CNRS France-Espagne Glycomimic: Oxocarbenium and glycosyl cations: from Chemistry to Enzyme
IC2MP – Institut de Chimie des Milieux et Matériaux de Poitiers, Poitiers (France)
13/June/2022 – 15/June/2022
Computational study of glucosyl and galactosyl cations in different environments: gas-phase, superacid and enzymatic media (talk)
A. Nin-Hill, C. Rovira

First Annual HIMS (van't Hoff Institute for Molecular Sciences) Symposium
HIMS (van't Hoff Institute for Molecular Sciences, Amsterdam (The Netherlands)
15/June/2022
Mechanistic analysis of UDP-D-Glucuronic Acid 4-epimerase from Bacillus Cereus *by means of Molecular Dynamics* (poster)
O. Esquivias, A. Borg, J. Coines, B. Nidetzky, C. Rovira

Molecular Simulation 2022: Present, Past and Future
Hotel Villa San Giovanni, Erice (Italy)
25/June/2022 – 29/June/2022
Computer simulation of new reaction mechanisms in carbohydrate-active enzymes (CAZymes) (talk)
C. Rovira
Modeling Bifidobacterium bifidum*'s lacto-N -biosidase by means of Molecular Dynamics* (poster, awarded with prize)
I. Cuxart, J. Coines, O. Esquivias, M. Faijes, A. Planas, X. Biarnés, C. Rovira
Asparagine Tautomerization in Glycosyltransferase Catalysis. The Molecular Mechanism of Protein O-Fucosyltransferase 1 (poster)
B. Piniello, E. Lira-Navarrete, H. Takeuchi, M. Takeuchi, R. S. Haltiwanger, R. Hurtado-Guerrero, C. Rovira

30th International Carbohydrate Symposium
Virtual symposium (Brazil)
10/July/2022 – 15/July/2022
Modeling mechanisms of glycosylation reactions in CAZymes, hand-in-hand with experiments (plenary talk)
C. Rovira
The catalytic reaction mechanism of the β-galactocerebrosidase enzyme deficient in Krabbe disease (poster)
A. Nin-Hill, C. Rovira
Modeling Bifidobacterium bifidum'*s lacto-N -biosidase by means of Molecular Dynamics*
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B. Piniello, E. Lira-Navarrete, H. Takeuchi, M. Takeuchi, R. S. Haltiwanger, R. Hurtado-Guerrero, C. Rovira

Gordon Research Conference (Computational Chemistry): Multiscale Modeling of Complex Systems: Methods and Applications
Rey Don Jaime Grand Hotel, Castelldefels (Spain)
17/July/2022 – 22/July/2022
Development and Application of the Nonbonded Cationic Dummy Models Accounting for Ion-Induced Dipole Interactions (poster)
Q. Liao, A. Pabis, B. Strodel, L. Kamerlin, C. Rovira
Bottom-up Exploration of the Chemical Space: an Efficient Algorithm for Ligand Discovery in Ultra-large Virtual Screening Libraries (Poster)
Álvaro Serrano-Morrás; Marina Miñarro; Andrea Bertran-Mostazo; Arnau Comajuncosa; Adrià Cabello; Carme Labranya; Jordi Juárez; Patrick Aloy; Carles Galdeano; Xavier Barril.
Using Molecular Dynamics simulations with organic solvents/water mixtures to identify imidazoline I2 receptor binding sites
Ozaydin, B.; Griñán-Ferré, C.; Bagán, A.; Pallàs, M.; Escolano, C.; Juarez-Jiménez, J.; Curutchet, C.
Environment effects change FRET distributions in a fluorophore-tagged disordered protein
Gonzalo, D.; Juárez-Jiménez, J.; Curutchet, C.
Understanding cooperativity effects in the drug-dependent degradation of the Cereblon neosubtrate CK1α
Miñarro-Lleonar, M; Bertran-Mostazo, A; Duro, J; Barril, X; Juárez-Jiménez, J.
Elucidating the Isoform-Selectivity of AMPK Towards Direct Activators: The Importance of the Dynamics in the Structure-Activity Relationship (invited talk)
C. Estarellas
Domain dynamics enable the cholesterol transport through the NPC1L1 transporter (poster)
A. Valdivia, FJ. Luque, S. Llabrés
From Quantum Dynamics to Multiscale Modeling of Materials and Interfaces (invited talk)
C.Curutchet
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 solvents/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

IQTCUB Meeting 2022
Facultat de Química de la UB, Barcelona (Spain)
19/July/2022 – 20/July/2022
CAZymes reaction mechanisms via QM/MM simulations (talk)
A. Nin-Hill, C. Rovira
Mechanistic analysis of UDP-D-Glucuronic Acid 4-epimerase from Bacillus Cereus *by means of Molecular Dynamics* (poster)
O. Esquivias, A. Borg, J. Coines, B. Nidetzky, C. Rovira

Modeling Bifidobacterium bifidum*'s lacto-N -biosidase by means of Molecular Dynamics* (poster)
I. Cuxart, J. Coines, O. Esquivias, M. Faijes, A. Planas, X. Biarnés, C. Rovira
Asparagine Tautomerization in Glycosyltransferase Catalysis. The Molecular Mechanism of Protein O-Fucosyltransferase 1 (poster)
B. Piniello, E. Lira-Navarrete, H. Takeuchi, M. Takeuchi, R. S. Haltiwanger, R. Hurtado Guerrero, C. Rovira
Singlet-splitting & triplet-pair dissociation in D-A copolymers for intramolecular singlet fission
M. Fumanal
Searching for novel mechanisms targeting Influenza A hemagglutinin: Inhibition of fusion peptide release (talk)
A.Valdivia
Activator vs Inhibitor of β-isoforms of AMPK: Towards the understanding of enzymatic mechanism (poster)
K. Barmpidi, F. J. Luque, C. Estarellas
Molecular factors that regulate the biometabolites of the gut microbiome: The specific case of Choline Trimethylamine-Lyase (poster)
M. Gomez, C. Estarellas
Combining Quantum Mechanics and Machine Learning Methods: Theoretical Prediction of Physico-Chemical Parameters of Drug-Like Compounds (poster)
A.Iaia, A. Viayna, C.D. Altomare, F.J. Luque
Towards a structure-based design of antimalarials guided by a complete 3D model of Plasmodium falciparum Glucose-6-phosphate dehydrogenase-6-phosphogluconolactonase (poster)
D. Vilchez**,** A. Viayna, F. J. Luque
Influence of water on the stability of photoactive TiO_2 nanoparticles (invited talk)
Á. Morales-García
cell2mol: encoding chemistry to intèrpret crystallographic data (invited talk)
S. Vela
Identifying the Atomic Layer Stacking of Mo_2C by Probe Molecule Adsorption (poster)
A. Jurado, Á. Morales-García, F. Viñes, F. Illas
Computational Pourbaix Diagrams for MXenes: A Key Ingredient Toward Proper Theoretical Electrocatalytic Studies (poster)
M. López, F. Viñes, K. S. Exner, F. Illas
Single-Atom Catalysts Based on PtN_x Based on the Electrocatalytic Chlorine Evolution Reaction: A Theoretical Study (poster)
L. Meng, F. Viñes, F. Illas, S. H. Joo
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 solvents/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
Functionals benchmark for photophysical properties of pyranoflavylium derivatives (poster)
J.R. Souza, C. Curutchet, Y.A. Aoto, P. Homem-de-Mello
Highly Adiabatic Time-Optimal Quantum Driving at Low Energy Cost (poster)
Ll. Garcia-Gonzalo, J. M. Bofill, I. de P. R. Moreira and G. Albareda

Prediction of partition coefficients in systems of micelles by DFT calculations (pòster)
Saranjan, L.; Fuguet, E.; Nedyalkova, M.; Simeonov. V.; Mas, F.; Madurga, S.
Unveiling the phenylalanine congregation mechanism for a deep understanding of phenylketonuria disease (pòster)
Barazorda-Ccahuana, H.L.; Mas, F.; Madurga, S.
Constant pH simulations of coarse-grained model of flexible linear polyelectrolytes (pòster)
Naranjo, D.; Blanco, P.M.; Garcés, J.L.; Mas, F.; Madurga, S.
Alpha- and beta-synuclein: pH-dependent conformations? (pòster)
Privat, C.; Madurga, S.; Mas, F.; Rubio, J.
Understanding cooperativity effects in the drug-dependent degradation of the Cereblon neosubtrate CK1α (Keynote)
Miñarro-Lleonar, M; Bertran-Mostazo, A; Duro, J; Barril, X; Juárez-Jiménez, J.

Twenty years of metadynamics (CECAM)
CECAM-HQ-EPFL, Lausanne (Switzerland)
5/September/2022 – 8/September/2022
QM/MM metadynamics simulations of new reaction mechanisms (talk)
C. Rovira
Structural and mechanistic insights into the cleavage of clustered O-glycan patches-containing glycoproteins by mucinases of the human gut (talk)
Q. Liao, V. Taleb, C. Rovira, R. Hurtado-Guerrero

16th Red Española de Supercomputación Users Conference (RES)
CénitS - COMPUTAEX, Cáceres (Spain)
14/September/2022 – 15/September/2022
The Catalytic Reaction Mechanism of the β-Galactocerebrosidase Enzyme Deficient in Krabbe Disease (talk)
A. Nin-Hill, C. Rovira
Understanding cooperative effects in PROTAC-Mediated Ternary Complexes for Protein Degradation (Keynote).
Miñarro-Lleonar, M; Bertran-Mostazo, A; Duro, J; Barril, X; Juárez-Jiménez, J.

Modeling and design of molecular materials 2022
Faculty of Social Sciences of the University of Gdańsk, Gdańsk (Poland)
19/September/2022 – 22/September/2022
Computer simulation of mechanisms in glycoprocessing enzymes using QM/MM approaches (talk)
C. Rovira

14th Carbohydrate Bioengineering Meeting (CBM14)
Norefjell Ski & Spa, Norefjell (Norway)
25/September/2022 – 28/September/2022
Uncovering novel catalytic mechanisms in glycosidases with the help of computer simulation (talk)
C.Rovira

The International Solvay Institutes for Physics and Chemistry. From 2D to 3D Crystals: A Multi-Scale, Multi-Technique and Multi-System Approach of the Crystallization of Organic Molecules on Tailored Carbon Surface
Brussels (Belgic)
21-23/03/2022
Simulated microgravity conditions for materials synthesis' (talk)
J. Puigmarti-Luis (invited by Prof. Yves Geerts)

Flow Chemistry Summit 2022 – SELECTBIO
Boston, (United States)
17-18/03/2022
Exploiting controlled reaction-diffusion conditions for materials synthesis (talk)
J. Puigmarti-Luis

15th European School on Molecular Nanoscience
Tordesillas, (Spain)
Celebration date (format: 22-27/05/2022)
What can microfluidic technologies offer? (talk)
J. Puigmartí-Luis (invited by Prof. Eugenio Coronado)

Con Instituto de Nanociencia y Materiales de Aragón (INMA)
Zaragoza, (Spain)
07/06/2022
Microfluidic technologies for chemistry and materials engineering (talk)
J. Puigmartí-Luis (invited by Prof. Jesús Santamaria)

International Conference on Manipulation, Automation and Robotics at Small Scales (MARSS)
Toronto, (Canada)
25-29/07/2022
MOFBOTS: Metal-Organic Framework-Based Biomedical Microrobots (talk)
J. Puigmartí-Luis (invited by Prof. S. Pané)

Beijing Institut of Technology (BIT)
Beijing (China)
02/08/2022
From molecules and assemblies to functional materials by design via microfluidic technologies (talk)
J. Puigmartí-Luis (invited by Prof. Muhua Huang)

University of Burgos
Burgos (Spain)
9-12/11/2022
Microfluidic technologies as an advanced tool for chemistry and materials synthesis (talk)
J. Puigmartí-Luis (invited by Prof. Tomás Torroba)

Cong Technical University of Dresden
Dresden (Germany)
20-21/11/2022
Microfluidic technologies as an advanced tool for chemistry and materials synthesis (talk)
J. Puigmartí-Luis (invited by Prof. Juliane Simmchen)

C2022 MRS Fall Meeting & Exhibit
Boston (United States)
27/11 – 2/12/2022
MOFBOTS: Metal–organic framework-based biomedical magnetic microrobots (talk)
J. Puigmartí-Luis (invited by Prof. S. Pané)

BOSS XVII, 17th Belgian Organic Synthesis Symposium
Namur (Belgica)
30/June/2022
Design, synthesis and biological activities of new purines and azapurines
Miquel Viñas; Jaume Ginard; Jaime Rubio; M. Dolors Pujol

PTI-Salud Global CONFERENCE
Valencia (España)
5/October/2022
Discovery of new inhibitors and mechanisms of inflammasome activation: applications in COVID-19
Pons, Mònica; Zodda, Erika; Calvo, Cristina; Benítez, Cristina; Rebollo, Elena; Raich, Dalia; Pérez, Daniel; Lama, Raquel; Maestro, David; Cascante, Marta: Villar, Ana; Novoa, Beatriz; Serrano, Anna; Rubio, Jaime; Izquierdo, Nuria; Thomson, Timothy

8th EuChemS Chemistry Congress
Lisboa (Portugal)
28/August/2022
Computational discovery of compounds against Parkinson disease through pharmacophore directed docking
Víctor Giménez-Oya, Ana Cañuelo, Jaime Rubio-Martínez, José M. Granadino-Roldán
Cage–···Cage– interaction: Boron cluster-based noncovalent bond and its applications in solid-state materials (talk)
J. Poater

Computer Simulation and Theory of Macromolecules 2022
Hünfeld Alemania)
8/April/2022
Accelerating the detection of allosteric sites in FBDD
Maria Nuria Peralta Moreno; Jaime Rubio Martinez; José Manuel Granadino Roldán

23rd EuroQSAR: European Symposium on Quantitative Structure-Activity Relationship
Heidelberg (Germany)
Celebration date (26/September/2022)
Bottom-up Exploration of the Chemical Space: an Efficient Algorithm for Ligand Discovery in Ultra-large Virtual Screening Libraries (Poster)
Álvaro Serrano-Morrás; Marina Miñarro; Andrea Bertran-Mostazo; Arnau Comajuncosa; Adrià Cabello; Carme Labranya; Jordi Juárez; Patrick Aloy; Carles Galdeano; Xavier Barril
Development of computational methods for rational design of minimal-size PROTACs (miniPROTACs) (Poster)
Patricia Blanco-Gabella; Alexander Gmeiner; Jordi Juárez-Jiménez; Xavier Barril.
Assessing the Suitability of 3D QM-Derived Atomic Hydrophobicity Patterns for Ligand-Target Interactions (invited talk)
F.J. Luque

12th Congress on Electronic Structure Principles and Applications (ESPA-2022) & Biannual Meeting of the GEQC

Vigo (Spain)

21-24/06/2022

Using Molecular Dynamics simulations with organic solvents/water mixtures to identify imidazoline I2 receptor binding sites

Ozaydin, B.; Griñán-Ferré, C.; Bagán, A.; Pallàs, M.; Escolano, C.; Juarez-Jiménez, J.; Curutchet, C.

Environment effects change FRET distributions in a fluorophore-tagged disordered protein

Gonzalo, D.; Juárez-Jiménez, J.; Curutchet, C.

Optimizing the thermodynamics and kinetics of the triplet-pair dissocia-tion in donor-acceptor copolymers for intramolecular singlet fission

M. Fumanal, C. Corminboeuf

Electronic structure of realistic C-doped anatase TiO_2 nanoparticles from first principles: Implications for photocatalysis (poster)

E. R. Remesal, Á. Morales-García, F. Illas

cell2mol: encoding chemistry to intèrpret crystallographic data (poster)

S. Vela

Determination of the energy ladder in cryptophyte photosynthetic antenna complexes from multiscale simulations (talk)

G.B. Ozaydin, C. Curutchet

Using Molecular Dynamics simulations with organic solvents/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

Functionals benchmark for photophysical properties of pyranoflavylium derivatives (poster)

J.R. Souza, C. Curutchet, Y.A. Aoto, P. Homem-de-Mello

Time-optimal quantum driving in a time-dependent drift Hamiltonian (poster)

Ll. Garcia-Gonzalo, J. M. Bofill, I. de P. R. Moreira and G. Albareda

Electronic structure and magnetic coupling in selenium substituted pyridine-bridged bisdithiazolyl multifunctional molecular materials (poster)

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

Controlling Chemical Reactivity with Optimally Oriented Electric Fields: A Generalisation of the Newton Trajectory Method (talk)

J. M. Bofill

XII Trobada de Joves Investigadors dels Països Catalans

Girona

24/01/2022-26/01/2022

Commutadors moleculars basats en canvis conformacionals de grups aril dipolars controlats per camp elèctric (talk)

K. Jutglar Lozano

Estudi de l'empaquetament cristal·lí de cadenes alifàtiques llargues

E. Colomer, P. Alemany

Vietnam-Taiwan Joint Symposium on Applied Science and Emergent 2D Materials (ASEM 2022)
Ho Chi Minh City, Vietnam
27/04/2022-29/04/2022
Mechanical control of the electronic states in 2D covalent organic frameworks (invited talk)
J. Ribas

Jujols X meeting. European Workshop on Theoretical Approaches of Molecular Magnetism
Roz Armor Village Vaccances, Erquy, France
30/05/2022-03/06/2022
Molecular orbital descriptor approach (MODA): A machine learning descriptor based on first principles to forecast magnetic couplings in organic magnets (talk)
R. Santiago, M. Deumal, J. Ribas
Solid-state effects on the singlet-triplet energy gaps of switchable diradicals
J. Ribas
Chairwoman in session 3 *(and* attendance*)*
M. Deumal
Evidence for low-lying correlated gapped states in strained graphene and graphenic 2D-COFs (Talk)
I. de P. R. Moreira

Virtual Conference on Chemistry and its Applications (VCCA)
University of Mauritius, Reduit, Maurici
08/08/2022-12/08/2022
Versatility on organic-inorganic hybrids: structures and properties *(poster)*
M. Rademeyer, B.M.P. Beebeejaun-Boodoo, E.M. van der Merwe, S.N. Bothma, S. Coetzee, N. Hearne, T. Mak, H.J. van der Poll, C.P. Landee, M.M. Turnbull, J.C. Monroe, R.M. Erasmus, J.J. Novoa, M. Deumal and F. Xiao

Northeast Regional Meeting (NERM) of ACS
The Joseph A. Floreano Rochester Riverside Convention Center, Rochester NY, USA
02/10/2022-05/10/2022
Copper(II) complexes of pyrazine-1,4-dioxide: chains and layers *(talk)*
R. Rodríguez Pérez, C.P. Landee, L.N. Dawe, M. Deumal, D.A. Dickie, M.M. Turnbull

Institut Germans Trias - Hospital Can Ruti (Spain)
Celebration date (format: 13/09/2022)
Targeting the nitrosative defense mechanism of Mycobacterium tuberculosis (invited seminar).
F.J. Luque.

Novartis (Switzerland)
Celebration date (format: 28/10/2022)
QM Continuum Solvation-Based Tools for the Study of the Bioactive Species of Drug-Like Compounds (invited seminar).
F.J. Luque.

University Californa Davis (U. S. A.)
Celebration date (format: 18/06/2022)
HYPHAR: A journey from continuum solvation models to virtual screening in drug discovery (invited seminar; online).
F.J. Luque.

17th German Conference on Cheminformatics - EuroSAMPL
Garmisch-Partenkirchen (Germany)
Celebration date (format: 08-12/05/2022)
Reliability of the IEFPCM-MST continuum solvation model in the SAMPL blind challenge (invited talk)
F.J. Luque.

From early discovery to translational medicinal chemistry". XX National Meeting of the Spanish Society of Medicinal Chemistry (SEQT)
Faculty of Medicine, University of Santiago, Santiago de Compostela (Spain)
Celebration date (format: 19-22/06/2022)
Remodeling of the conformational landscape of the Aβ42 toward off-pathway aggregates (talk)
F.J. Luque.
Elucidating the selectivity for β-isoforms of direct allosteric modulators of AMPK: disclosing clues for improving drug design (talk)
C. Estarellas, K. Barmpidi, E. Aledavood, F.J. Luque.
Activator vs Inhibitor of β-isoforms of AMPK: Towards the understanding of enzymatic mechanism (poster)
K. Barmpidi, F.J. Luque, C. Estarellas.

ACS Spring 2022, Bonding Through Chemistry
San Diego (U. S. A.)
Celebration date (format: 20-24/03/2022)
Decoding allosterism in AMPK regulation: Towards the design of isoform-selective activators (invited talk)
F.J. Luque.
Boron Cluster Based Non-Covalent Cage-···Cage- Interaction (talk)
Survival of the aromaticity in boron clusters despite radical structural changes (talk)
J. Poater

XXVII National Meeting on Medicinal Chemistry
Bari (Italy)
Celebration date (format: 11-14/09/2022)
Combining quantum mechanics and machine learning in the search of the bioactive conformation of drug-like compounds (talk)
A. Viayna, A. Iaia, C. D. Altomare, F. J. Luque

5th European Workshop on AMPK and AMPK-related kinases
Golden Jubilee Conference Hotel, Glasgow (UK)
Celebration date (format: 26-29/09/2022)
Towards the understanding of isoform selectivity by direct activators (talk)
C. Estarellas, F.J. Luque

International Bioinformatics Conference, IBC'2022
Kenzie Salozur Hotel, Tanger (Morocco)
Celebration date (format: 09-10/10/2022)
Understanding the structure-action relationship of Choline Trimethylamine-Lyase for developing novel therapeutic strategies of cardiovascular diseases (Invited talk)
C. Estarellas

International hydride Conference on Oxygen Binding and Sensing Proteins (O2BiP)
Golden Jubilee Conference Hotel, Rome (Italy)
Celebration date (format: 6-9/09/2022)
Targeting a putative reductase partner of the truncated hemoglobin N in Mycobacterium tuberculosis (poster)
K. Barmpidi**,** E. Aledavood, F. Issoglio, D. A. Estrín, C. Estarellas, F. J. Luque

The 14th International Conference on Quantum Fluid Clusters
Erice (Italy)
19/04/2022-22/04/2022
Vibrational relaxation of a diatomic molecule in a superfluid helium nanodroplet: influence of the nanodroplet size, interaction energy and energy gap (oral communication)
M. Blancafort, A. Vilà, M. González
Recombination is important in the photodissociation of Br_2(B) in superfluid helium nanodroplets (poster)
A. Vilà, M. González

Ciclo de seminarios 2021/2022 del Departamento de Química Física de la UCM
Instituto de Cerámica y Vidrio, Madrid (Spain)
24/05/2022
Crystal facet engineering for tailoring photoactive TiO_2 nanoparticles (invited talk)
Á. Morales-García

Erasmus Mundus Master in Sustainable Chemistry
University of Poitiers, Poitiers (France)
1-2/12/2022
Computational Methods and Models in Modern Heterogeneous Catalysis - Vols. I-IV (invited talk)
F. Viñes
13-14/01/2022
Computational Chemistry in Heterogeneous Catalysis - Vols. I-IV (invited talk)
F. Viñes

LVIII Congreso Nacional de la SECV
Instituto de Cerámica y Vidrio, Madrid (Spain)
04/05/2022
Identificación del apilamiento de capas de las fases MXenes: Mo_2C como caso de estudio (talk)
A. Jurado, Á. Morales-García, F. Viñes, F. Illas
MXenes para tecnologías de captura, almacenamiento y conversión de CO_2 (keynote talk)
F. Viñes, Á. Morales-García, F. Viñes, F. Illas

NANOWS 2022 – Achievements and challenges of multiscale modelling of nanocrystals for eficient wàter splitting
University of Aveiro, Aveiro (Portugal)
11-12/07/2022
Understanding the influence of water on the properties of photoactive titania nanoparticles (invited talk)
Á. Morales-García

II Meeting of the UB Institutes
University of Barcelona, Barcelona (Spain)
23/09/2022
Novel Carbon Capture, Storage, and Use Technologies from First Principles Calculations (invited talk)
F. Viñes

V Tesimarató de Química
Universitat de Barcelona, Facultat de Química, Barcelona (Spain)
22/11/2022
Metanació del CO_2 en materials MXenes (talk)
D. Dolz, F. Viñes, Á. Morales-García
Estudi computacional de tendències de catalitzadors metàl·lics per reaccions clau mediambientals (talk)
D. Vázquez-Parga, F. Viñes, Á. Morales-García

III Premi de Pòsters de Sostenibilitat i Drets Humans
Universitat de Barcelona, Barcelona (Spain)
22/11/2022
Systematic Study, from First Principles Calculations, of the Adsorption and Dissociation of Probe CO Molecule on low Miller Indices Transition Metal Surfaces (poster)
D. Vázquez-Parga, F. Viñes
Grazynes: New 2D Materials for Biogas Upgrading (poster)
A. Calzada, F. Viñes, P. Gamallo

Psi-k Conference
SwissTech Convention Center, Lausanne (Switzerland)
22-25/08/2022
cell2mol: encoding chemistry to intèrpret crystallographic data (poster)
S. Vela
Clar π-Sextet Rule Determines Aromaticity and Extrusion of Benzenoids Linked to [o-COSAN]− (talk)
J. Poater

Triennial Congress of the World Association of Theoretical and Computational Chemists Applications (WATOC 2022)
Vancouver (Canada)
3-8/07/2022
Grazynes: carbon-based 2D composites with exotic properties and applications (talk)
P. Gamallo, A. Calzada, F. Viñes, R. Sayós
Grazynes: carbon-based 2D composites with exotic properties and Applications
Invited talk
P. Gamallo, A. Calzada, F. Viñes, R. Sayós

Ni clusters supported on TiC(001) boost the activity towards the CO_2 hydrogenation reaction: a kinetic Monte Carlo study
Pòster
P. Lozano, H. Prats, F. Illas, R. Sayós

9th Young Scientist Workshop on Theoretical Chemistry and Computational Modelling
University of Vigo, Vigo (Spain)
21-24/06/2022
Environment effects change FRET distributions in a fluorophore-tagged disordered protein (talk)
D. Gonzalo, J. Juárez-Jiménez, C. Curutchet

I Jornada acadèmica del programa de doctorat de Recerca, Desenvolupament i Control de Medicaments
University of Barcelona, Barcelona (Spain)
1/07/2022
Multiscale modelling of light harvesting and photoinduced processes in biosystems (talk)
G.B. Ozaydin, J. Juárez-Jiménez, C. Curutchet

XIII Jornada de Recerca a la Facultat de Farmàcia i Ciències de l'Alimentació
University of Barcelona, Barcelona (Spain)
19/10/2022
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 solvents/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
Functionals benchmark for photophysical properties of pyranoflavylium derivatives (poster)
J.R. Souza, C. Curutchet, Y.A. Aoto, P. Homem-de-Mello

26th International Congress of Chemical and Process Engineering (CHISA 2022)
Praga (República Txeca)
21-25/08/2022
Learning Analytics Introduction in the Chemical Engineering Subject of the Chemistry Undergraduate Degree of the University of Barcelona for the Teaching/Learning/Assessment Process Improvement.
A.E. Plesu, E. Ramírez, J. Bonet, J.H. Badia, R. Soto, M. Iborra.

1st International Scientific Conference on Cleaner Energy and Chemical Engineering for Sustainable Circular Economy (CLES-CE 2022)
Sofia (Bulgaria)
28-31/08/2022

Assessment on the Circular Economy Processes of Pha Production from Municipal Organic Wastes Through Acidogenic Fermentation.
K. Cheah, J. Dosta, A.E. Plesu Popescu, J. Bonet-Ruiz.
Novel Process for Aqueous Mea-CO_2 Hydrogenation to Methanol Using Reactive Distillation.
A.E. Plesu Popescu, E. Meco, J. Bonet-Ruiz, J. Llorens

25th conference on Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction (PRES'22)
Bol (Croacia)
5-8/09/2022
Sampling of Porous Materials for Post-Combustion Capture of CO_2 Based on GCMC Simulations.
P. Gamallo, J. Cardenas Gamboa, R. Sayós, X. Gimenez.
A Kinetic Dft-Based Theoretical Study of CO_2 Hydrogenation on Ni (111): Kinetic Monte Carlo vs. Microkinetic Modelling.
A. Gracia, P. Lozano, P. Gamallo, F. Huarte-Larrañaga, R. Sayós.
Optimised Separation Process of Ketones from Biomass Pyrolysis Oil.
V. Manso, J. Bonet-Ruiz, D. Curcó, J. Llorens, A.E. Plesu Popescu.
Recovery of valuable solvents from the pharmaceutical industry wastewater.
V. Manso, A. Hamad Piqué, J. Bonet-Ruiz, D. Curcó, A.E. Plesu Popescu.
Biofuel Butyl Levulinate Synthesis in a Heterogenous Catalytic Distillation.
M.A. Tejero, A.E. Plesu Popescu, J.H. Badia, J. Bonet-Ruiz, J. Tejero.
Gas Immission Assessment Charts Based on Computational Fluid Dynamics Simulations.
R. Cabello, C. Troyano Ferré, A.E. Plesu Popescu, J. Bonet-Ruiz, D. Curcó, J. Llorens.

VI Congreso de Innovación Docente en Ingeniería Química (VI CIDIQ)
Madrid (España)
11-13/07/2022
Introducción de analíticas de aprendizaje en la asignatura de Ingeniería Química del grado de Química de la Universidad de Barcelona.
E. Ramírez Rangel, A.E. Plesu Popescu, J. Bonet Ruiz.

XII National and III International Conference on Engineering Thermodynamics (CNIT 12)
Madrid (España)
29/06/2022 – 01/072022
Understanding the thermo-physical properties of nanofluids.
Svobodova-Sedlackova; A. Calderón; M. Majó; C. Barreneche; P. Gamallo; A. I. Fernández

11th Singapore International Chemistry Conference
Singapore (Singapore)
11/12/2022
Aromaticity and extrusion of benzenoids linked to [o-COSAN]-: Clar has the answer (invited talk)
J. Poater

4th Workshop on Magnetically Induced Currents in Molecules (MAGIC2022)
Cambridge (UK)
11/09/2022
Persistent strong diatropic ring currents in aromatic closo- and nido-carboranes (invited talk)
J. Poater

9th European Conference on Boron Chemistry
Barcelona (Spain)
03/07/2022
Aromaticity in boron clusters survives radical structural changes (talk)
J. Poater

Royal Society Hooke Discussion Meeting: Supercomputer modelling of advanced materials
The Royal Society, London (UK)
Celebration date (format: day/month/year)*From Gomberg to graphene and beyond: new multifunctional 2D materials based on persistent radicals (Invited talk)*
S. T. Bromley

Collision Physics and Chemistry and their Applications Conference, COPCA 2022
Valletta (Malta)
Nanosilicate Dust in the Interstellar Medium: Theory, Experiment and Obervation *(Invited talk)*
S. T. Bromley

6th Energy Materials workshop - Modelling Energy Interfaces
The Thomas Young Centre, London (UK)
An Unconstrained Approach to Systematic Structural and Energetic Screening of Materials Interfaces *(Talk)*
S. T. Bromley

MasterQuímica XVII
Venue, Barcelona (Spain)
Celebration 24-26/05/2022
Recuperació de nitrogen amoniacal en purins de porc utilitzant una membrana permeable al gas (pòster)
Ben Hammou-Abboud, Y.; Serra-Toro, A.; Astals, S.; Mas, F.; Dosta, J.
Modelització computacional d'una solució d'àcids húmics (pòster)
Naranjo, D.; Blanco, P.M.; Garcés, J.L.; Mas, F.; Madurga, S.

META 2022: XIV Congreso de la Mesa Española de Tratamiento de Aguas
Venue, Sevilla (Spain)
Celebration date 1-3/06/2022
Recuperación del nitrógeno de un efluente de fermentación acidogénica mediante una membrana permeable al gas (pòster)
Serra-Toro, A.; Astals, S.; Mas, F.; Dosta, J.

CORFU 2022: 9th International Conference on Sustainable Solid Waste Management
Corfu (Greece)
Celebration date 15-18/06/2022
Recovery of ammonia from acidogenic fermentation effluents using a hydrophobic membrane contactor (talk, oral communication)
Serra-Toro, A.; Vinardell, S.; Astals, S.; Llorens, J.; Mata-Álvarez, J.; Mas, F.; Dosta, J.

ESMO Congress
París (France)
Celebration date: 9-13/09/2022
A new clinically applicable immune-metabolic signature (IMMETCOLS) reveals metabolic singularities in Consensus Molecular Subtypes (CMS) in colorectal cancer (pòster))
Madurga, S.; Foguet, C.; Oliveres, H.; Mas, F.; Maurel, J.; Cascante, M.

SEOM22
Madrid (Spain)
Celebration date: 18-21/10/2022
Una nueva firma inmuno-metabólica (IMMETCOLS) muestra singularidades metabólicas entre los subtipos moleculares de consenso (CMS) en cáncer colorrectal (talk, oral communication)
Gorria, T.; Madurga, S.; Foguet, C.; Oliveres, H.; Mas, F.; Maurel, J.; Cascante, M.

ESPA 2022
Vigo (Spain)
21-24/06/2022
Crystal Packing of Long Aliphatic Chains
L. Sánchez, E. Colomer, P. Alemany
Computational study of the molecular packing in crystalline polyethylene using DFT-based methods with van der Waals functionals
E. Colomer, L. Sánchez, P. Alemany
Cosymlib: a Python library for continuous symmetry measures
F. Jiménez-Cuélliga, M. Llunell. E. Bernuz, A. Carreras, P. Alemany

RESEARCH STAYS IN RECOGNIZED CENTERS

Sven Krüger

TU München, Munich (Germany)

Konstantin Neyman

April 2022

Maytal Caspary Toroker

Technion, Haifa (Israel)

Konstantin Neyman

May 2022

Bernd Ensing, associate profesor

HIMS (van't Hoff institute for Molecular Sciences, Amsterdam (The Netherlands)

Oriol Esquivias Bautista de Lisbona, Universitat de Barcelona

March 2022 – July 2022

Prof. Michail Stamatakis

University College London(UCL), London (UK)

Daniel Dolz García, University of Barcelona

February-April 2022

Prof. Alberto Roldán Martínez

Cardiff University, Cardiff (Wales)

David Vázquez Parga, University of Barcelona

February-April 2022

Jaime Llanos

Universidad Católica del Norte, Antofagasta (Chile)

Pere Alemany, Universitat de Barcelona

May 2022

Abel Carreras

Donostia International Physics Cahner, Donostia (

Pere Alemany, Universitat de Barcelona

June 2022

Jaime Llanos

Universidad Católica del Norte, Antofagasta (Chile)

Pere Alemany, Universitat de Barcelona

November-December 2022

PARTICIPATION IN COMPETITIVE FUNDED RESEARCH PROJECTS

Development and application of grand canonical global optimization methods.
A.Bruix, Universitat de Barcelona
La Caixa Foundation Junior Leader, 2022-2025
La Caixa Foundation – Junior Leader Programme
305.000 €

Computational modelling of complex materials for advanced technologies
P. Alemany, K. Neyman, Universitat de Barcelona
PID2021-128217NB-I00, 2022-2025
MCIUN
108.900€

Estructura electrónica y propiedades de moléculas y sólidos
P. Alemany, K. Neyman, Universitat de Barcelona
PGC2018-093863-B-C22, 2019-2022
MCIUN
12.100€

Unidad de excelencia «María de Maeztu» para INSTITUT DE QUIMICA TEORICA I COMPUTACIONAL
F. Illas, E. Ruiz, IQTCUB, Universitat de Barcelona
MDM-2017-0767, 2018-2022
MCIUN
2.000.000€

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
40.000€

Development of a computational platform for kinetic studies of complex nanostructured catalysts. - Beatriu de Pinós grant for Dr. Albert Bruix Fusté
K. Neyman, Universitat de Barcelona
2018BP00190, 2020-2023 (terminated in 2022; switching to a more prestigious laCaixa grant)
AGAUR, Generalitat de Catalunya
144.300€

Pre-doctoral FPI grant for Pablo Castro Latorre
K. Neyman, Universitat de Barcelona
PRE2019-088979, 2021-2025
MICIN
98.250€

Pre-doctoral FPI grant for Riccardo Farris
K. Neyman, Universitat de Barcelona
PRE2020-091903, 2021-2025
MICIN
98.960€

HPC-Europa3 grant for Boris Merinov (Caltech, USA)
K. Neyman, Universitat de Barcelona
HPC17QU8IV, 03/2022-04/2022
HPC-Europa3, supported by the European Commission H2020 Research & Innovation GA # 730897

HPC-Europa3 grant for Sergey Kozlov (National University of Singapore, Singapore)
K. Neyman, Universitat de Barcelona
HPC17BVAIN, 11/2021-01/2022
HPC-Europa3, supported by the European Commission H2020 Research & Innovation GA # 730897

HPC-Europa3 grant for Elena Zerbato (University of Trieste, Italy)
K. Neyman, Universitat de Barcelona
HPC1777CT3, 03/2022-04/2022
HPC-Europa3, supported by the European Commission H2020 Research & Innovation GA # 730897

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€

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 €

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€

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
MICIN N
Amount: 120.000€

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€

Training interdisciplinary glycoscientists to get a molecular-level grip on glycocodes at the human mucosa–microbiota interface
T. Wennekes (Utrecht University, NL), N. Juge (Quadram Institute, UK), H. Overkleeft (Leiden University, NL), A. Molinaro (University of Naples Federico II, Italy), A. Salonen (University of Helsinki, Finland), C. Rovira (Universitat de Barcelona), P. Cani (University of Louvain, Belgium), J. Beauprez (Inbiose & Ghent University, Belgium), L. Vigsnæs (Glycom & Technical University Denmark, Denmark), A. Mercenier (Nutrileads & Utrecht University, NL), R. Field (Iceni Diagnostics & University East Anglia, UK)
H2020-MSCA-ITN-2018-SWEET CROSSTALK, 2019-2022
EU
Amount (corresponding to UB): 250.904,88 €

SGR-Cat 2021 SGR 00270.
J. Puigmartí-Luis, Universitat de Barcelona
SGR 00270, 2022-2025
Financing entity (AGAUR)
Amount: 36.000€

EVA: ME 3D printing technology – the revolution of actuatable composites
J. Puigmartí-Luis, Universitat de Barcelona
101047081, 2022-2026
HORIZON-EIC-2021-PATHFINDEROPEN-01 (EU)
2.109.624 €:

Synthesis and controlled growth of metal-organic frameworks with microfluidic technologies
J. Puigmartí-Luis, Universitat de Barcelona
PID2020-116612RB-C33, 2021-2023
Agencia Estatal de Investigación (MINECO)
150.000 €

MAgnetically steerable wireless Nanodevices for the tarGeted delivery of therapeutIc agents in any vascular rEgion of the body (ANGIE).
J. Puigmartí-Luis, Universitat de Barcelona
952152, 2021-2025
European Commission (EU)
4.000.000 €

New approaches to nano-engineer MOF films for electronic and biotechnology applications (M-O-Films).
J. Puigmartí-Luis, Universitat de Barcelona
2019-2022
Nanosciences Foundation: (Université Grenoble Alpes)
351.000 €:

Functional 2D porous crystalline materials (2DMats).
J. Puigmartí-Luis, Universitat de Barcelona
2019-2023
Swiss National Founds
600.000 CHF:

Ultra-versatile Structural PRINTing of amorphous and tuned crystalline matter on multiple substrates (SPRINT).
J. Puigmartí-Luis, Universitat de Barcelona
801464, 2020-2023
European Commission (EU)
2.999.997,50 € (435,375.00 € to ETH Zürich)

Tuning Tubulin Dynamics and Interactions to Face Neurotoxicity: a Multidisciplinary Approach for Training and Research (TubInTrain).
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.
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 €

Discovery of small molecules to prevent the severe progression of COVID-19.
Marta Cascante Serratosa, Universitat de Barcelona
2020PANDE00048, 13/05/2021 -12/11/2022
AGAU - Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR)
349.000,00 €

Bases Moleculares de Cooperatividad Química en complejos ternarios de interés terápeutico
Jordi Juárez-Jimenez, Universitat de Barcelona
PID2020-115683GA-I00, 2021-2024
Financing entity (MINECO)
Amount: 99.400€

MATERIALES BASADOS EN MOLECULAS DE CAPA ABIERTA: COMPRENSION Y PREDICCION DE SUS ESTRUCTURAS Y PROPIEDADES FISICAS A TRAVES DE LA MODELIZACION COMPUTACIONAL
Jordi Ribas and Mercè Deumal, Universitat de Barcelona
PID2020-117803GB-I00, 2021-2024
MICINN
Amount: 121.000,00 €

Molecular Engineering of 2D Covalent Organic Frameworks for Optoelectronic Applications
Beatriu de Pinós fellowship to Maria Fumanal supervised by Jordi Ribas, Universitat de Barcelona
BP 2020 00050, full period 01/04/2022 to 31/03/2025, completed period 01/04/2022 to 31/12/2022
Agència de Gestió d'Ajusts Universitaris i de Recerca
Amount for three years: 144.300,00 €

Molecular Engineering of 2D Covalent Organic Frameworks for Optoelectronic Applications
Maria Fumanal, Universitat de Barcelona
QHS-2022-3-0014, 01/11/2022-28/02/2023
Red Española de Supercomputación (RES)
Amount: 432.000 computer hours

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 €

Towards an improvement in diagnostics and treatment strategies for TB control (ADVANCE- TB)
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: 56.806,15 €

OPen-shell ELectronic SYStems - OPELSYS
Mercè Deumal Solé, Universitat de Barcelona
2021 SGR 00354, 2022-2025
GENCAT
Amount: 40.000€

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
MICIN
Amount: 45.530 €

Computationally driven tuning up of novel bidimensional MXene catalysts for greenhouse gases reduction and hydrogen generation
Francesc Viñes & Carme Sousa, Universitat de Barcelona
PID2021-126076NB-I00, 2022-2025
MICIN
Amount: 169.400 €

Apoyo a la actividad científica de los grupos de recerca de Catalunya
Francesc Illas, Universitat de Barcelona
2021-SGR-00079, 2022-2024
AGAUR
Amount: 60.000 €

Computational materials science for eficient water splitting with nanocrystals from abundant elements
Francesc Illas (Leader WG1), Universitat de Barcelona
CA18234, 2019-2023
Financing entity (EU-COST)
Amount: 64.000 €

Computational Large-scale Characterization of Spin Crossover Molecular Switches. Towards an Atlas for Materials Discovery
Sergi Vela, Universitat de Barcelona
2020-BP-00043, 2022-2025
AGAUR
Amount: 144.000 €

ALLODD - Allostery in Drug Discovery - H2020-MSCA- ITN-2020
Zoe Curnia, Academy of Athens, Greece
Project 956314, 2021-2025
EU
Amount: 3.669.353,64€

Modelling the interplay between structure and spectroscopy in biosystems
Carles E. Curutchet, Universitat de Barcelona
PID2020-115812GB-I00, 2021-2024
MINECO
Amount: 96.800€

Química Computacional Aplicada para la captura, separación y conversión de CO_2 en combustibles ligeros.
Ramón Sayós, Pablo Gamallo, Universitat de Barcelona
RTI2018-094757-B-I00, 2018-2022(prorrogado)
MINECO
Amount: 85.426 €

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

Estudio Teórico y Espectroscópico de Moléculas Orgánicas Birradicalarias Relevantes para la Química Bioorgánica y los Materiales Moleculares Multifuncionales.
Josep Maria Bofill, Universitat de Barcelona
PID2019-109518GB-I00, 2020-2022
MINECO
Amount: 60.500€

Diseño Computacional de Electrocatalizadores Hibridos de Metal-Radical Organico para Reacciones de Importancia Socioeconomica y Ambiental
S. T. Bromley & F. Calle Vallejo, Universitat de Barcelona
PID2021-127957NB-I00, 2022-2025
MICIN
Import: 163.350€

Electrocatalysts based on Redox Active Self Assembled Monolayers
S. T. Bromley & F. Calle Vallejo, Universitat de Barcelona
TED2021-132550B-C21, 2022-2025
MICIN
Import: 132.480€

Nuevas estrategias computacionales para el estudio de agregación y adsorción de microplásticos y nanoplásticos a contaminantes en medios acuáticos naturales
Haruna Luz Barazorda Ccachuana (Universidad Católica Santa María, Arequipa, Perú), Sergio Madurga (UB), Francesc Mas (UB)
151-2020-FONDECYT. Fondo Nacional de Desarrollo Tecnológico e Innovación Tecnológica, 2020-2023
Amount: 45.550€

Ammonia recovery from animal slurries by means of a novel selective membrane.
J. Mata Álvarez, F. Mas, University of Barcelona
Private company contract, 2021-2023
INDUKERN-REVAGO
Amount: 88.354€

Identificación de los subtipos metabólicos de cáncer colorrectal para el desarrollo de medicina personalizada
Marta Cascante Serratosa; Pedro Ramon de Atauri Carulla
PID2020-115051RB-I00 - Programa Nacional de Biomedicina- Ministerio de Ciencia e Innovación (MICINN), 2021-2024
Amount: 411.800€

Grup de Bioquímica Integrativa
Marta Cascante Serratosa
2021 SGR 0350 SGRC - Ajuts de Suport als Grups de Recerca de Catalunya (SGR)- Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR), 2022-2025
Amount: 60.000€

Integración de membranas permeables al amoníaco y bioreactores anaeróbicos de membrana para producir fertilizantes y biogás a partir de aguas residuales de alta carga
TED2021-132422B-I00. NTME - Programa Nacional de ciencias y tecnologías medioambientales. MCNN - Ministerio de Ciencia e Innovación (MICINN), 2022-2024.
Joan Dosta Parras; Sergi Astals Garcia (Enginyeria Química, UB)
Amount: 195.500€

Una estrategia integral para valorizar residuos procedentes de granjas porcinas mediante la producción de recursos valiosos para el sector alimentario.(VALPIG4FOOD)
TED2021-129595B-I00. NTME - Programa Nacional de ciencias y tecnologías medioambientales. MCNN - Ministerio de Ciencia e Innovación (MICINN), 2022-2024.
Daniel Puyol Santos (Universidad Rey Juan Carlos, Madrid)
Amount: 184.000€

PATENT OR MARK APPLICATION

Compounds affecting KRAS
Agell Jané, Nieves; Pujol Dilmé, Maria; Rubio Martínez, Jaime; Jaumot Pijoan, Montserrat; Garrido Sagarzazu, Eduardo; Vilaplana Saiz, Marta; Abuasaker, Baraa; Brun Lozano, Sonia ***Application number:*** *EP22383292.4*
Fecha Solicitud / Prioridad *27/12/2022*

Quantum control
Titular/s: Ll. Garcia, J.M. Bofill, I. de P.R. Moreira, G. Albareda
Application number: PCT/EP2022/088078

Institut de Química Teòrica i Computacional