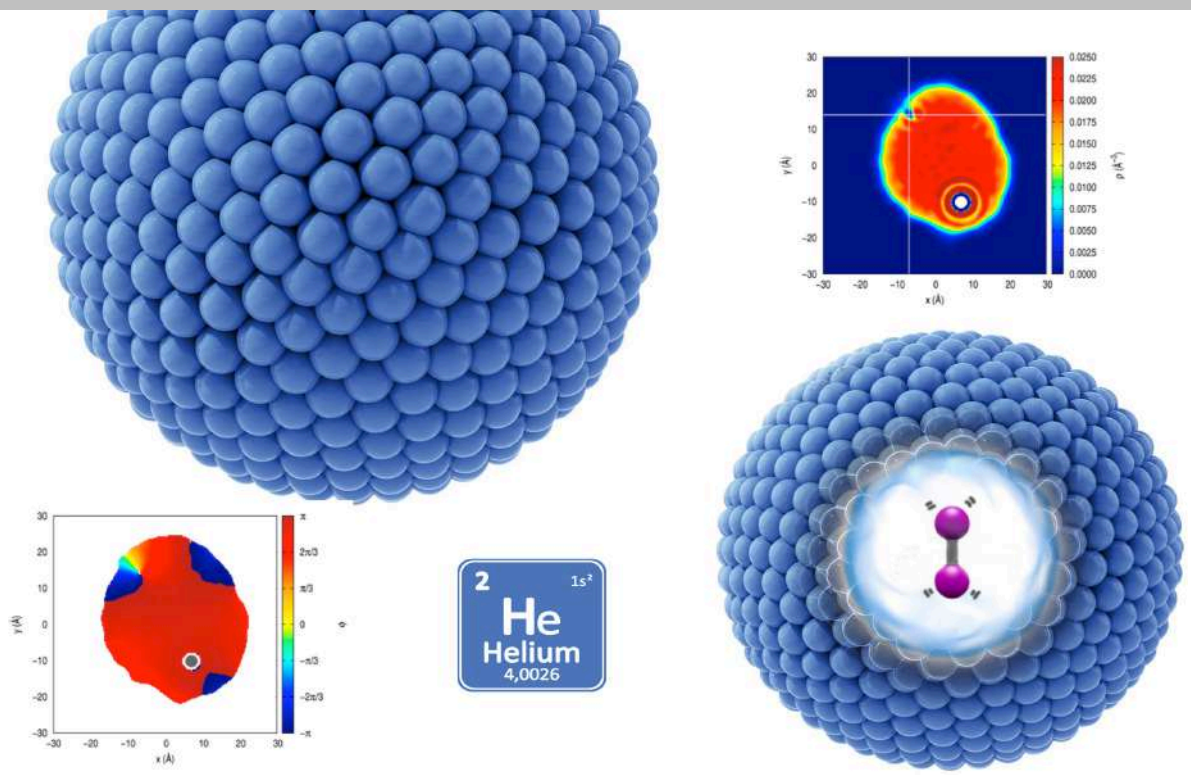
Institut de Química Teòrica
i Computacional
UNIVERSITAT DE BARCELONA

UNIVERSITAT DE BARCELONA

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

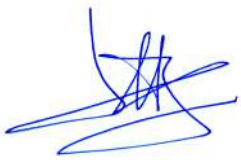



## Activity Report 2018

La creació de l'Institut de Química Teòrica i Computacional de la Universitat de Barcelona (IQTCUB) va ser aprovada al Consell de Govern en sessió ordinària el 21 de novembre de 2007. Des de l'abril del 2018 tinc l'honor de ser-ne el Director. Vull aprofitar aquesta oportunitat d'encapçalar la memòria anual de l'IQTCUB per agrair explícitament als Drs. Francesc Illas, Ramón Sayós i Carme Rovira per haver participat a l' anterior equip de direcció de l'IQTCUB i també al Dr. Jordi Poater per incorporar-se al costat del Prof. Francesc Illas en el nou equip de direcció de l'Institut. Aquest 2018 ha estat important a causa de la incorporació de nous grups de la Facultat de Farmàcia (Drs. Carles Curuchet i Javier Luque). Així mateix, des del punt de vista de reconeixement extern la concessió de l'ajut de María de Maeztu ha de suposar un salt tant en la qualitat com en la quantitat de la investigació realitzada en el nostre Institut. Aquest fet hauria també de produir una incorporació de nous membres a l'Institut que aportin tant un augment de la qualitat de la nostra investigació com una diversificació en els temes dels nostres projectes de recerca.

L'objectiu comú dels projectes de recerca duts a terme a l'Institut és l'ús de mètodes arrelats a la química quàntica, recentment també està obert a grups experimentals dels nostres departaments amb estretes col·laboracions amb grups de recerca centrats en Química Computacional. Això ha de fomentar i augmentar el caràcter multidisciplinari de la nostra recerca. Tradicionalment, la recerca de l'IQTCUB es distingeix del que hom espera d'un químic tradicional, ja que el instruments emprats pels nostres investigadors no es troben en un laboratori típic sinó potser en un "laboratori" de càlcul que sovint només és el punt d'entrada als nostres recursos computacionals o a centres de supercomputació amb capacitat de càlcul encara més gran.

L'objectiu principal de la Química Teòrica i Computacional és aconseguir una comprensió detallada dels processos químics i físics per ajudar a interpretar els resultats experimentals i fer prediccions que condueixin a nous experiments. En fer-ho, aquesta disciplina pot aportar nous conceptes que permetin avançar en el disseny racional de nous materials amb propietats físiques i la seva aplicació en dispositius electrònics i magnètics, al descobriment de nous fàrmacs i a comprendre processos bioquímics, a noves reaccions que proporcionen una millora dels processos químics per fer-los més eficaços i més respectuosos amb el medi ambient i proposar noves fonts d'energia sostenibles, per afrontar els reptes que actualment té la nostra societat. A més, hem d'integrar en la nostra recerca noves eines com l'aprenentatge automàtic (intel·ligència artificial), la realitat virtual i nous recursos informàtics (computació "exascale" i quàntica).



Eliseo Ruiz
Director de l'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

Two direction teams have joined IQTCUB during 2018. The outgoing team,

| | |
|---|---|
| **Prof. Francesc Illas Riera** | *Director* |
| **Prof. Ramón Sayós Ortega** | *Treasurer and Secretary* |
| **Prof. Carme Rovira Virgili** | *Board member* |

and the incoming team,

| | |
|---|---|
| **Prof. Eliseo Ruiz Sabin** | *Director* |
| **Prof. Jordi Poater Teixidor** | *Secretary* |
| **Prof. Iberio de P. Ribeiro Moreira** | *Treasurer* |
| **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 four main research lines.

1. **Methods, algorithms and computational tools development**

Here we focus on theories and algorithms devoted to account for electronic correlation, nuclear motion, quantum structure-activity, continuous symmetry measures, molecular modelling, variational state transition theory and magnetic resonance. Further developing of Monte Carlo, molecular dynamics and Brownian dynamics is also envisaged.

2. **Computational Materials Science**

In this research area we employ computational methods, ranging from high-level quantum chemistry and ab initio molecular dynamics to classical simulation methods, to investigate the bulk, surface and nanoscale properties of a broad class of solid materials, such as complex inorganic compounds, molecular crystals and heterogeneous catalysts.

3. **Computational Biochemistry and Soft Matter**

Using the arsenal of available computational methods, from electronic structure based methods to classical simulations, we focus on systems of biological interest. In particular we investigate the structure and reactivity of proteins and enzymes, drug design, processes in cellular membranes, enzymatic reactions in crowded media and soft nanoparticles in solution.

4. **Reactivity and Reaction Dynamics**

Research in this area uses quantum, classical and statistical mechanics methods to analyse the dynamics of elementary reactions, electronic excited states and atmospheric and combustion reactions. Continuum methods are also used to investigate macromolecular complexation reactions in aqueous media.

## I.3 IQTCUB MEMBERS

IQTCUB involves a total of 90 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 | Department/Unit | Section |
|---|---|---|---|
| **Full Professors** | | | |
| Aguilar Navarro | Antonio | Materials Science & Physical Chemistry | Physical Chemistry |
| Alemany i Cahner | Pere | Materials Science & Physical Chemistry | Physical Chemistry |
| Alvarez Reverter | Santiago | Inorganic and Organic Chemistry | Inorganic Chemistry |
| Bofill Villà | Josep Maria | Inorganic and Organic Chemistry | Organic Chemistry |
| González Pérez | Miguel | Materials Science & Physical Chemistry | Physical Chemistry |
| Illas Riera | Francesc | Materials Science & Physical Chemistry | Physical Chemistry |
| Luque Garriga | Francisco J. | Nutrition, Food Sciences & Gastronomy | Basic Sciences |
| Mas Pujadas | Francesc | Materials Science & Physical Chemistry | Physical Chemistry |
| Novoa Vide | Juan José | Materials Science & Physical Chemistry | Physical Chemistry |
| Rubio Martínez | Jaime | Materials Science & Physical Chemistry | Physical Chemistry |
| Ruiz Sabin | Eliseo | Inorganic and Organic Chemistry | Inorganic Chemistry |
| Sayós Ortega | Ramón | Materials Science & Physical Chemistry | Physical Chemistry |
| **Associate Professors** | | | |
| Costa Sala | Ramón | Inorganic and Organic Chemistry | Inorganic Chemistry |
| D. P. Ribeiro Moreira | Ibério | Materials Science & Physical Chemistry | Physical Chemistry |
| Giménez Font | Xavier | Materials Science & Physical Chemistry | Physical Chemistry |
| Huarte Larrañaga | Fermín | Materials Science & Physical Chemistry | Physical Chemistry |
| Lucas Alcorta | Josep Maria | Materials Science & Physical Chemistry | Physical Chemistry |
| Llunell Marí | Miquel | Materials Science & Physical Chemistry | Physical Chemistry |
| Mota Valeri | Fernando | Materials Science & Physical Chemistry | Physical Chemistry |
| Paniagua Valle | Juan Carlos | Materials Science & Physical Chemistry | Physical Chemistry |
| Solé Sabaté | Albert | Materials Science & Physical Chemistry | Physical Chemistry |
| Sousa Romero | Carme | Materials Science & Physical Chemistry | Physical Chemistry |
| Vilaseca Font | Eudald | Materials Science & Physical Chemistry | Physical Chemistry |

**Other Categories (Professors Agregats)**

| | | | |
|---|---|---|---|
| Aullón López | Gabriel | Inorganic and Organic Chemistry | Inorganic Chemistry |
| Bonet Ruiz | Jordi | Chem. Engineering & Analytical Chem. | Chem. Engineering |
| Curutchet Barat | Carles E. | Pharm. & Pharm. Tech. & Phys. Chem. | Physical Chemistry |
| Deumal Solé | Mercè | Materials Science & Physical Chemistry | Physical Chemistry |
| Díez Pérez | Ismael | Materials Science & Physical Chemistry | Physical Chemistry |
| Gamallo Belmonte | Pablo | Materials Science & Physical Chemistry | Physical Chemistry |
| Madurga Díez | Sergio | Materials Science & Physical Chemistry | Physical Chemistry |
| Ribas Ariño | Jordi | Materials Science & Physical Chemistry | Physical Chemistry |
| Reigada Sanz | Ramón | Materials Science & Physical Chemistry | Physical Chemistry |

**Other Categories (Professors Associats)**

| | | | |
|---|---|---|---|
| Bahamón | Daniel | Chem. Engineering & Analytical Chem. | Chem. Engineering |
| Bidon-Chanal Badia | Axel | Nutrition, Food Sciences & Gastronomy | Basic Sciences |
| Cirera Fernández | Jordi | Inorganic and Organic Chemistry | Inorganic Chemistry |
| Corbella Morató | Marina | Pharm. & Pharm. Tech. & Phys. Chem. | Physical Chemistry |
| Jover Modrego | Jesús | Inorganic and Organic Chemistry | Inorganic Chemistry |
| López Marne | Estefanía | Materials Science & Physical Chemistry | Physical Chemistry |
| Piqué Caufapé | Oriol | Materials Science & Physical Chemistry | Physical Chemistry |
| Prats García | Hèctor | Materials Science & Physical Chemistry | Physical Chemistry |
| Tercero Mohedano | Javier | Inorganic and Organic Chemistry | Inorganic Chemistry |
| Valero Montero | Rosendo | Materials Science & Physical Chemistry | Physical Chemistry |

**ICREA Research Professors**

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

**Postdoctoral contracts**

*Beatriu de Pinós-Juan de la Cierva*

| | | | |
|---|---|---|---|
| Echeverría López | Jorge | Inorganic and Organic Chemistry | Inorganic Chemistry |
| Morales García | Ángel | Materials Science & Physical Chemistry | Physical Chemistry |
| Wang | Binju | Inorganic and Organic Chemistry | Organic Chemistry |

*Marie-Curie*

| | | | |
|---|---|---|---|
| Albareda Piquer | Guillem | IQTCUB | |

*Ramón y Cajal*

| | | | |
|---|---|---|---|
| Calle Vallejo | Federico | Materials Science & Physical Chemistry | Physical Chemistry |
| Viñes Solana | Francesc | Materials Science & Physical Chemistry | Physical Chemistry |

*Contracte Projecte de Recerca*

| | | | |
|---|---|---|---|
| Bahamón | Daniel | Materials Science & Physical Chemistry | Physical Chemistry |
| Estarellas Martín | Carolina | Nutrition, Food Sciences & Gastronomy | Basic Sciences |
| Ginex | Tiziana | Nutrition, Food Sciences & Gastronomy | Basic Sciences |
| Kshatresh Dutta | Dubey | Inorganic and Organic Chemistry | Organic Chemistry |
| Valero Montero | Rosendo | Materials Science & Physical Chemistry | Physical Chemistry |

*Other*

| | | | |
|---|---|---|---|
| Cortijos Aragonès | Albert | Materials Science & Physical Chemistry | Physical Chemistry |
| De Souza Pinheiro | Silvana | Pharm. & Pharm. Tech. & Phys. Chem. | Physical Chemistry |
| Vega Pallauta | Mauricio | Inorganic and Organic Chemistry | Inorganic Chemistry |
| Vilà Casanova | Arnau | Materials Science & Physical Chemistry | Physical Chemistry |

**Ph.D. Students**

*FI Grant (Catalan Government Program)*

| | | | |
|---|---|---|---|
| Aledavood | Elnaz | Nutrition, Food Sciences & Gastronomy | Basic Sciences |
| Balcells Nadal | Cristina | Materials Science & Physical Chemistry | Physical Chemistry |
| Blanco Andrés | Pablo Miguel | Materials Science & Physical Chemistry | Physical Chemistry |
| Nin Hill | Alba | Inorganic and Organic Chemistry | Organic Chemistry |
| Vega Domínguez | Lorena | Materials Science & Physical Chemistry | Physical Chemistry |

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

| | | | |
|---|---|---|---|
| Bernuz Fitó | Efrem | Materials Science & Physical Chemistry | Physical Chemistry |
| Coines López-Nieto | Joan | Inorganic and Organic Chemistry | Organic Chemistry |
| Martín Rodríguez | Alejandro | Inorganic and Organic Chemistry | Inorganic Chemistry |
| Piñero Vargas | Juan José | Materials Science & Physical Chemistry | Physical Chemistry |
| Posada Pérez | Sergio | Materials Science & Physical Chemistry | Physical Chemistry |

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

| | | | |
|---|---|---|---|
| Alcon Rovira | Isaac | Materials Science & Physical Chemistry | Physical Chemistry |
| Amoza Dávila | Martín | Inorganic and Organic Chemistry | Inorganic Chemistry |
| Mondelo Martell | Manel | Materials Science & Physical Chemistry | Physical Chemistry |
| Vilaplana Saiz | Marta | Materials Science & Physical Chemistry | Physical Chemistry |

*ITN UE Grant*

| | | | |
|---|---|---|---|
| Cuko | Andi | Materials Science & Physical Chemistry | Physical Chemistry |
| Francese | Tommaso | Materials Science & Physical Chemistry | Physical Chemistry |

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

| | | | |
|---|---|---|---|
| Alonso Benito | Gerard | Materials Science & Physical Chemistry | Physical Chemistry |
| Blancafort Jorquera | Miquel | Materials Science & Physical Chemistry | Physical Chemistry |
| Macià Escatllar | Antoni | Materials Science & Physical Chemistry | Physical Chemistry |
| Roncero Barrero | Cristina | Materials Science & Physical Chemistry | Physical Chemistry |
| Svobodova | Adela | Materials Science & Physical Chemistry | Materials Science |
| Velásquez Benites | Juan Diego | Inorganic and Organic Chemistry | Inorganic Chemistry |

*Beca CONICYT*

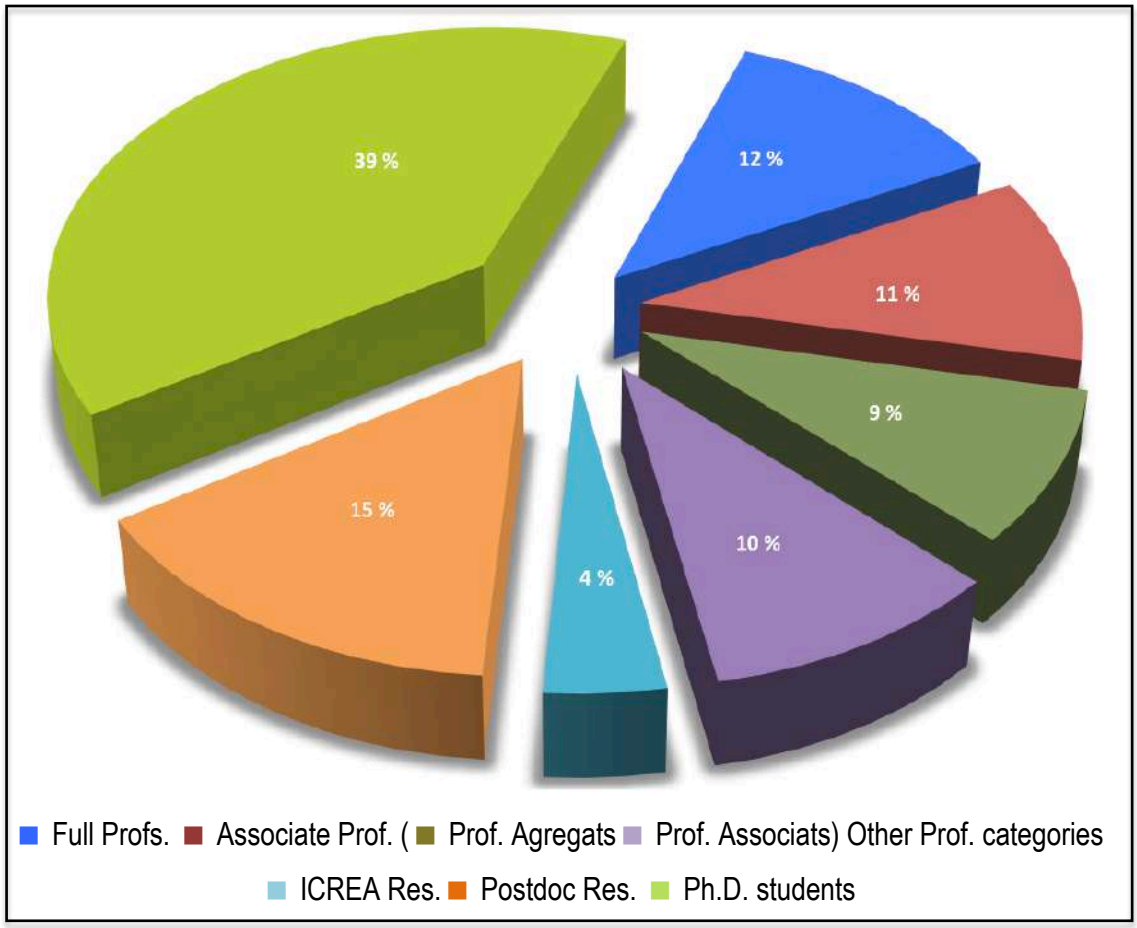
| | | | |
|---|---|---|---|
| Zamora | William J. | Nutrition, Food Sciences & Gastronomy | Basic Sciences |

*Beca Doctorat Industrial*

| | | | |
|---|---|---|---|
| Vázquez López | Javier | Nutrition, Food Sciences & Gastronomy | Basic Sciences |

*Other*

| | | | |
|---|---|---|---|
| Costas Viñas | Pol | Materials Science & Physical Chemistry | Physical Chemistry |
| De Moya | Natalia | Materials Science & Physical Chemistry | Physical Chemistry |
| Figueras Valls | Marc | Materials Science & Physical Chemistry | Physical Chemistry |
| Jurado Mañas | Anabel | Materials Science & Physical Chemistry | Physical Chemistry |
| Kamalinahad | Saedeh | Materials Science & Physical Chemistry | Physical Chemistry |
| Kassiani | Motaki | Materials Science & Physical Chemistry | Physical Chemistry |
| López Berbel | Martí | Materials Science & Physical Chemistry | Physical Chemistry |
| Lozano Reis | Pablo | Materials Science & Physical Chemistry | Physical Chemistry |
| Morales Salvador | Raúl | Materials Science & Physical Chemistry | Physical Chemistry |
| Privat Contreras | Cristian | Materials Science & Physical Chemistry | Physical Chemistry |
| Raich Armendáriz | Lluís | Inorganic and Organic Chemistry | Organic Chemistry |
| Santiago Piera | Raúl | Materials Science & Physical Chemistry | Physical Chemistry |
| Seira | Constantí | Nutrition, Food Sciences & Gastronomy | Basic Sciences |
| Viayna | Antonio | Nutrition, Food Sciences & Gastronomy | Basic Sciences |
| Vila Julià | Guillem | Ciència de Materials i Química Física | Química Física |
| Vílchez | David | Nutrition, Food Sciences & Gastronomy | Basic Sciences |




Distribution of IQTCUB members according to the professional category.

## I.4 TECHNICAL STAFF

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

| | |
|---|---|
| **Jordi Inglés Camats** | *System Administrator Manager* |
| **Teresa Arenal Porcel** | *System Administrator* |

## I.5 EQUIPMENT

Currently, the IQTCUB computational facilities consist of nine calculation clusters located in two conditioned rooms of the Chemistry and Physics Faculty of UB. All the clusters except iqtc06 and iqtc07 are in a room near the garage of the faculty where it is cooled by two air conditioning machines of 47,000 and 66,000 KW, respectively. Iqtc06 and Iqtc07 are located in a room called VAX, which is cooled by one air conditioner machine of 30,000 KW and another two of 9,000KW.

### CALCULATION CLUSTERS

**cerqt2** (*invested value 400.000 €*)

| | |
|---|---|
| *Machine type* | SUN cluster (4 racks) |
| *Operating system* | SLES10 |
| *Services* | *Calculation cluster and disk server (raid of 2.5TB)*. Internal DHCP server |
| *Structure* | Master + 111 nodes |
| *Notes* | There are heterogeneous nodes with 32 and 64 bits processors. |

*Specifications:*

**Master**
CPU: 1,80 GHz Opteron Dual processor (64bits)
RAM: 8 GB
HD: 1 x 146 GB hard disk + 2,5 TB direct attached storage
Network: 2 gigabit network cards (one for external network and one for calculation network)

**7 Sun Fire V60X nodes (3,06 GHz processor)**
CPU: 3,06 GHz Xeon Dual processor (32 bits)
RAM: 3 GB
HD: 2 x 36 GB hard disk
Network: 2 gigabit network cards (calculation network)

**92 Sun Fire V60X nodes (2,80 GHz processor)**
CPU: 2,80 GHz Xeon Dual processor (32 bits)
RAM: 6 nodes with 4 GB, 86 nodes with 3 GB
HD: 2 x 36 GB hard disk
Network: 2 gigabit network cards (calculation network)

**11 Sun Fire V20Z nodes (1,80 GHz processor)**
CPU: 1,80 GHz Opteron Dual processor (64 bits)
RAM: 10 nodes with 8 GB, 2 nodes with 16 GB
HD: 10 nodes with 2 x 73 GB hard disk, 2 nodes with 2 x 73GB and 2 x 300 GB hard disk respectively
Network: 2 gigabit network cards (calculation network)

**1 Sun Fire V20Z node 64 bits (2,20 GHz processor)**
CPU: 2,20 GHz Opteron Dual processor (64 bits)
RAM: 16 GB
HD: 2 x 146 GB hard disk
Network: 2 gigabit network cards (calculation network)

**iqtc01** (*invested value 250.000 €*)

| | |
|---|---|
| *Machine type* | HP cluster |
| *Operating system* | Debian Stable |
| *Services* | Calculation cluster |
| *Structure* | 80 nodes |
| *Notes* | 64 bits processors |

*Specifications:*

**80 AMD HP ProLiant DL145 G2 nodes**
CPU: 2 x 2,2 GHz AMD Opteron 275 Dualcore
RAM: 8 GB
HD: 2 x 80 GB hard disk
Network: 2 gigabit network card (calculation network) + 1 ILO card (out of band network, OOB)

**iqtc02** (*invested value 78.000 €*)

| | |
|---|---|
| *Machine type* | HP cluster |
| *Operating System* | SLES10 |
| *Services* | Calculation cluster |
| *Structure* | 26 nodes |
| *Notes* | 64 bits processors |

*Specifications:*

**17 INTEL HP ProLiant DL160 G5 nodes**
CPU: 2 x 2,66 GHz Xeon QuadCore
RAM: 16 GB
HD: 2 x 250 GB hard disk
Network: 2 gigabit network card (calculation network) + 1 ILO card (OOB)

**5 INTEL HP ProLiant DL160 G5 nodes**
CPU: 2 x 2,66 GHz Xeon QuadCore
RAM: 16 GB
HD: 4 x 250 GB hard disk
Network: 2 gigabit network card (calculation network) + 1 ILO card (OOB)

**1 INTEL HP ProLiant DL160 G5 node**
CPU: 2 x 2,66 GHz Xeon QuadCore
RAM: 16 GB
HD: 2 x 500 GB hard disk
Network: 2 gigabit network card (calculation network) + 1 ILO card (OOB)

**3 INTEL HP ProLiant DL160 G5 nodes**
CPU: 2 x 2,66 GHz Xeon QuadCore
RAM: 32 GB
HD: 2 x 250 GB hard disk
Network: 2 gigabit network card (calculation network) + 1 ILO card (OOB)

**iqtc03** (*invested value 33.000 €*)

| | |
|---|---|
| *Machine type* | HP cluster |
| *Operating System* | SLES10 |
| *Services* | Calculation cluster |
| *Structure* | 11 nodes |
| *Notes* | 64 bits processors. Merged with iqtc02 cluster |

*Specifications:*

**11 INTEL HP ProLiant DL140 G3 nodes**
CPU: 2 x 2,33 GHz Xeon QuadCore
RAM: 16-32 GB
HD: 2 x 80 GB hard disk
Network: 2 gigabit network card (calculation network) + 1 ILO card (OOB)

**iqtc04** (*invested value 460.000 €*)

| | |
|---|---|
| *Machine type* | HP cluster |
| *Operating system* | SLES11 |
| *Services* | Calculation cluster |
| *Structure* | 101 nodes |
| *Notes* | 64 bits processors. Infiniband network |

*Specifications:*

**95 INTEL HP ProLiant DL160 G6 nodes**
CPU: 2 x 2,66 GHz Xeon SixCore
RAM: 48 GB
HD: 1 x 1 TB hard disk
Network: 2 gigabit network card (internal data network) + 2 infiniband network (calculation network) + 1 ILO card (IAM)

**4 INTEL HP ProLiant DL160 G6 nodes**
CPU: 2 x 2,66 GHz Xeon SixCore
RAM: 48 GB
HD: 4 x 500 GB hard disk
Network: 2 gigabit network card (internal data network and calculation network) + 1 ILO card (OOB)

**2 INTEL HP ProLiant DL160 G6 nodes**
CPU: 2 x 2,66 GHz Xeon SixCore
RAM: 48 GB
HD: 1 x 500 GB hard disk
Network: 2 gigabit network card (internal data network and calculation network) + 1 ILO card (OOB)

**iqtc05** (*invested value 32.000 €*)

| | |
|---|---|
| *Machine type* | SGI Cluster |
| *Operating System* | SLES11 |
| *Services* | Calculation cluster |
| *Structure* | 4 nodes |
| *Notes* | 64 bits processors |

*Specifications:*

**4 AMD SGI H2106-G7 nodes**
CPU: 4 x 2,3 GHz Opteron 6276 16-core
RAM: 256 GB
HD: 2 x 1 TB hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (OOB)

**iqtc06** (*invested value 420.000 €*)

| | |
|---|---|
| *Machine type* | Heterogeneous Cluster |
| *Operating System* | SLES11 |
| *Services* | Calculation cluster |
| *Structure* | 32 nodes |
| *Notes* | 64 bits processors |

*Specifications:*

**25 INTEL HP ProLiant DL560 Gen8 nodes**
CPU: 4 x 2,2 GHz Xeon OctoCore
RAM: 512 GB
HD: 2 x 300 GB hard disk
Network: 4 gigabit network card (calculation network) + 1 IPMI card (OOB)
Network: 2 x 10 gigabit network card (internal data network)

**7 INTEL Supermicro SuperServer 8017R-TF+**
CPU: 4 x 2,3 GHz Xeon OctoCore
RAM: 512 GB
HD: 3 x 1 TB hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (OOB)
Network: 2 x 10gigabit network card (internal data network)

**iqtc07** (*invested value 40.000 €*)

| | |
|---|---|
| *Machine type* | Supermicro Cluster |
| *Operating System* | SLES12 |
| *Services* | Calculation cluster |
| *Structure* | 2 nodes |
| *Notes* | 64 bits processors |

*Specifications:*

**2 Supermicro 2048U RT4 nodes**
CPU: 4 x 2,6 GHZ Intel Broadwell 10Core
RAM: 512 GB or 1 TB
HD: 1 x 1 TB hard disk
Network: 4 gigabit network card (calculation network) + 1 IPMI card (OOB)
Network: 2 x 10gigabit network card (internal data network)

**iqtc08** (*invested value 155.000 €*)

| | |
|---|---|
| *Machine type* | HP Cluster |
| *Operating System* | Centos 7.2 |
| *Services* | Calculation cluster |
| *Structure* | 21 nodes |
| *Notes* | 64 bits processors |

*Specifications*

**21 HP Proliant DL360 Gen9**
CPU: 2 x 2,6 GHz Intel Xeon E5-2690 v4 14-core
RAM: 768 GB
HD: 1 x 1 TB hard disk
Network: 4 gigabit network card (calculation network) + 1 IPMI card (OOB)
Network: 2 x 10gigabit network card (internal data network)

**GPU cluster** (*invested value 57.000 €*)

*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

## SERVERS

**Glusterfs disk server** (*invested value 30.000 €*)

| | |
|---|---|
| *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)

**Portal (user access servers)** (*invested value 2.300 €*)
*Machine type* 2 redundant HP ProLiant DL120 G5 nodes
*Operating system* Debian stable
*Services* SGE Execution Host, Heartbeat, ssh server
*Structure* 2 redundant nodes
*Notes* User access servers for submitting jobs and accessing user data. Critical service connected with a UPS

*Specifications:*

**2 INTEL HP ProLiant DL120 G5 node**
CPU: 1 x 2,33 GHz Xeon Dual Core
RAM: 8 GB
HD: 1 x 160 GB hard disk
Network: 2 gigabit network card (internal network)

**Virtualization servers** (*invested value 18.300 €*)

| | |
|---|---|
| *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)

**Graphical applications server** (*invested value 3.000 €*)

| | |
|---|---|
| *Machine type* | 1 HP ProLiant DL385 node |
| *Operating system* | Debian Stable |
| *Services* | Server for the use of graphical applications (gaussview, p4vasp, etc.) |
| *Structure* | 1 node |
| *Notes* | Server connected to an UPS |

*Specifications:*

**1 AMD HP ProLiant DL385 node**
CPU : 2 x 2,2 GHz AMD Opteron 275 Dualcore
RAM: 4 GB
HD: 6 x 146 GB hard disk
Network: 1 10/100 network (external network) + 1 gigabit network (internal network)

## OTHERS

The IQTCUB have other services to provide service to the IQTCUB's users.

1. Backup server DELL R515 (backup server with 4TB of disk capacity connected to a UPS).
2. Tape library server HP MSL4048 (48 tapes with approximately 48TB of space, ~1TB/tape).
3. Administration server (laptop with 3 network cards for critical incidences support).
4. Proxy server (server that allows the access to the public network from IQTCUB's network).
5. Switch Layer 3 HP Procurve with 24 ports (used for the IQTCUB's date centre infrastructure).
6. 8 Switchs Layer 2 Dlink with 48 ports (internal network for cerqt2, iqtc01, iqtc02, iqtc03 clusters).
7. 4 Switchs Layer 2 HP with 48 ports (internal network for iqtc04, iqtc05 and iqtc06 cluster).
8. 3 Switchs Infiniband Voltaire with 36 ports (calculation network for iqtc04 cluster).
9. Modular switch HP (8 calculation network modules for iqtc01, iqtc02, iqtc03 clusters).
10. 2 Modular switch HP 10GB (calculation network for iqtc06 and data network for the glusterfs servers).
11. 2 Switch Netgear XS728T 10GB (internal and calculation network for iqtc08).
12. 1 Switch HPE 1810-24 (internal network iqtc08).

The approximated invested cost of this equipment is *50.000 €.*

## SUMMARY

Cores ..... 3,994 c

Memory ..... 27,816 GB RAM

Calculation disk capacity ..... 199 TB

Data user disk capacity ..... 32 TB

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

*2.028.000 €**

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

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

# II. IQTCUB ACTIVITIES

## II.1 GENERAL ACTIVITIES

Next, a description of activities and actions promoted by IQTCUB through 2017 is provided.

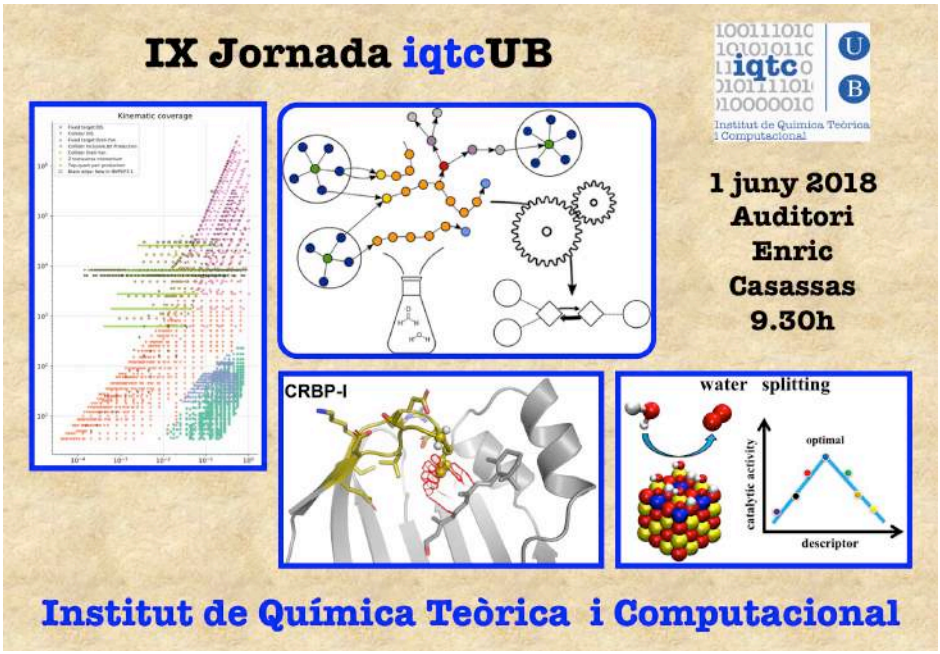
a. ***Promotion and encouragement of research.*** This year the IQTCUB has finally offered three contracts (around 2000 € per contract) aimed to help students to initiate a scientific career. These contracts are addressed to students about to end the degree and aimed to cover a six-month period to facilitate the student to pursue an official Master at UB as well as collaborating in some of the research projects of the IQTCUB groups. The contract has been awarded to Anabel Jurado Mañas and Raúl Morales Salvador for starting Master studies under the supervision of Dr. Francesc Viñes, and to Beatriz Piniello Castillo for starting it under the supervision of Dr. Carme Rovira.

*Total cost: 6.246 €*


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

b. ***9th IQTCUB workshop.*** This one-day workshop aimed at the dissemination of the research done at the IQTCUB took place on June 1st, 2018 at it was organized by Prof. Mercè Deumal and Dr. Jordi Cirera. The IQTCUB members and internationally acknowledged speakers present the most recent work. This year we highlight the participation of Prof. Dr. Markus Reiher from the ETH of Zurich with the invited lecture entitled *Authomated and Interactive Exploration of Complex Reaction Mechanism*, and Prof. Dr. José Ignacio Latorre from Institut de Ciències del Cosmos of UB with the invited lecture entitled *Quantum Disruption*. Moreover, Dra. Carol Estalleras (*Self-Controlled Ligand Release Mechanism as Determinant of the Selective Retinol Binding to Celular Carriers*), Dr. Federico Calle-Vallejo (*Computational Design of New Materials for Water Electrolyzers*) and Mr. Martín Amoza Dávila (*Understanding the Origin of Magnetic Anisotropy in S=1/2 Mononuclear Transition Metal Complexes*) from Universitat de Barcelona and IQTCUB gave us some details about their research. 14 poster contributions have been presented during the meeting. The IQTCUB assigned a budget to cover the traveling and lodging expenses of Prof. Dr. Markus Reiher as well as the catering service offered to all assistants.

*Total cost: 1.728 €*




Panel of the *9th IQTCUB workshop*.

c. ***8th Introductory course in Computational Chemistry.*** The main goal of this course organized by Prof. Gabriel Aullón member of the Inorganic and Organic Chemistry Department and the IQTCUB, is to initiate chemistry undergraduate students in the possibilities of Computational Chemistry. The course takes place during a whole week and is mainly addressed to Chemistry and Chemical Engineering students at the University of Barcelona. The 2018 edition has been the eighth one and 10 students have participated. The different issues exposed along with the teaching staff involved in each session was the following:

1. *Introduction to Linux*, Oriol Lamiel and Antoni Macià (UB, IQTCUB).
2. *Visualising Biomolecules,* Drs. Carme Rovira, Alba Nin, Joan Coines and Binju Wang (UB, IQTCUB).
3. *Structured Programming,* Profs. Albert Solé and J. Carlos Paniagua (UB, IQTCUB).
4. *Cellular Automaton,* Prof. Pere Alemany and Efrem Bernuz (UB, IQTCUB).
5. *Simulation of diffusion by means of Monte Carlo techniques*, Prof. Sergio Madurga (UB, IQTCUB).
6. *Computer Modelling of Materials,* Dr. Stefan Bromley *(UB, IQTC).*
7. *Analysing molecular properties by means of Computational Chemistry Tools,* Prof. Gabriel Aullón (UB, IQTCUB).

The present edition took place from June 25th to 29th.

*Total cost: 250 €*

d. ***7th Advanced Course in Computational Chemistry.*** Fuelled by the positive feedback received from the students in the previous editions we have offered again this year a course at a more advanced level with the main goal of improving previous knowledge in use of computers and on Computational Chemistry. Profs. Jaime Rubio and Miguel González from the Materials Science and Physical Chemistry Department of University of Barcelona and IQTCUB have organized the course that has been held in June 25rd to 29th. The participants in the course are usually students who have taken part in the Introductory Course or Chemistry undergraduates who have followed a Quantum Chemistry course. In this edition 7 students performed the registration: O. Piqué, M. López, A. Palacios, L. Vega, A. Cardenal, G. Murrià i C. Outeda. IQTCUB has covered breakfast catering expenses of all participants.

*Total cost: 240 €*

The different issues exposed along with the teaching staff have been the following:

1. *Introducció SGE,* Gerard Alonso (UB, IQTCUB).
2. *Estats excitats,* Prof. Mercè Deumal (UB, IQTCUB).
3. *Reaccions en fase gas: dinàmica i cinètica,* Profs. Miguel Gonzalez i Pablo Gamallo (UB, IQTCUB).
4. *Simulacions de Monte Carlo Cinèticen catàlisi heterogènia*, Prof. Ramon Sayós i Hèctor Prats (UB, IQTCUB).
5. *stat sòlid,* Profs. Iberio Ribeiro (UB, IQTCUB).
6. *Fortran 90,* Prof. Miquel Llunell (UB, IQTCUB).
7. *Disseny de fàrmacs*, Prof. Jaime Rubio (UB, IQTCUB).
8. *Modelització multiescala de dissolucions i biomolècules*, Prof. Carles Curutxet (UB, IQTCUB).


Panel of the 7th *Advanced Course in Computational Chemistry* held in 2018.

Pictures showing the students that shared the *Advanced Course in Computational Chemistry*.

e. ***IQTC Internal Seminars.*** In 2018 the periodic *IQTC Internal Seminars* have continued. Those seminars are given in order to disseminate the different research lines of the IQTC groups. The organizers of these seminars are the Ph.D students Efrem Bernuz and Antoni Macià, both members of the IQTC and the Materials Science and Physical Chemistry Department of the University of Barcelona. Here it is the list of the seminars held during 2018:

1. *Ab initio study in low spin magnetic complexes: candidates for qubits.*
   Martín Amoza, 19 january 2018.
2. *Useful tools for computational chemistry.*
   Héctor Prats, 19 january 2018.
3. *A simple approach to connect experimental and computational electrocatalysis*.
   Dr. Federico Calle-Vallejo, 21 març 2018.
4. *Post-PhD project application.*
   Dr. Isaac Alcón, 10 may 2018.
5. *Coupling conformational and ionization equilibria to model polyelectrolyte stretching.*
   Pablo Blanco Andrés, 14 june 2018.
6. *Single-molecule electronic transport properties: magnetoresistance and switching behaviour.*
   Alejandro Martín Rodríguez, 14 june 2018.
7. *Modelling metal/metal-oxide interface effects in nanocomposite materials for catalysis and beyond.*
   Prof. Konstantin Neyman, 18 september 2018.
8. *Charge transport in bisdithiazolyl-based compounds.*
   Cristina Rocero, 16 october 2018.
9. *Disseny i síntesi de compostos organics amb potencial activitat antitumoral per inhibició enzimàtica.*
   Marta Vilaplana, 6 november 2018.
10. *Production and uses of hydrogen.*
    Juan José Piñero, 6 november 2018.
11. *On the description of transition metal systems by density functionals.*
    Lorena Vega, 11 december 2018.
12. *Tuning activity of transition metal carbides by surface metal alloying: case of study of $CO_2$ capture.* Martí López, 11 december 2018.

*f.* ***Scientific Dissemination Activities.*** Prof. Xavier Giménez Font has been involved in the following scientific and teaching dissemination activities during 2018:

1. "*UB s'Apropa 18*".
   Gresol International American School, Terrassa, 1 january 2018.
   INS Pius Font i Quer, Manresa, 10 january 2018.
   INS Celestí Bellera, Granollers, 11 january 2018.
   INS Miramar, Viladecans, 12 january 2018.
   INS Celestí Bellera, Granollers, 12 january 2018.
   INS Montserrat Miró i Vilà, Sta. Coloma Gramanet, 15 january 2018.
   INS Domènec Perramon, Arenys de Munt, 16 january 2018.
   INS La Vall del Tenes, Sta. Eulàlia de Ronsana, 16 january 2018.
   INS Pau Vila, Sabadell, 17 january 2018.
   INS Baix a Mar, Vilanova i la Geltrú, 22 january 2018.
   INS Domènec i Montaner, Canet de Mar, 24 january 2018.
   INS Celestí Bellera, Granollers, 25 january 2018.
   Escola Pia, Caldes de Montbui, 25 january 2018.
   Escola Pia, Granollers, 25 january 2018.
   Escola La Presentació, Arenys de Mar, 30 january 2018.
   Escola Goar, Viladecans, 31 january 2018.
   INS Torre de Malla, Parets del Vallès, 31 january 2018.
   INS Les Termes, Sabadell, 1 february 2018.
   INS Vilamajor, Sant Pere de Vilamajor, 1 february 2018.
   INS Cal Gravat, Manresa, 2 february 2018.
   Escola Andorrana de Batxillerat, La Margineda, Andorra, 8 february 2018.
   INS Sentmenat, Sentmenat, 14 february 2018.
   INS Vinyet, Sitges, 15 february 2018.
   INS Alba del Vallès, Sant Fost de Campsentelles, 27 february 2018.
   INS Guillem Catà, Manresa, 15 march 2018.
   INS Vescomtat Cabrera, Hostalric, 16 march 2018.
   INS Lliçà d'Amunt, Lliçà d'Amunt, 20 march 2018.
   INS Maria de Bell–Lloc, Bigues i Riells, 17 april 2018.
   Escola Pia Igualada, Igualada, 19 april 2018.

2. Coarse "*L'Aire que respirem, l'energi que ens mou*"
   Universitat Popular, Caldes de Montbui, 10 january 2018.
   Universitat Popular, Caldes de Montbui, 24 january 2018.
   Universitat Popular, Caldes de Montbui, 31 january 2018.
   Universitat Popular, Caldes de Montbui, 7 february 2018.
   Universitat Popular, Caldes de Montbui, 14 february 2018.
   Universitat Popular, Caldes de Montbui, 21 february 2018.
   Universitat Popular, Caldes de Montbui, 28 february 2018.
   Universitat Popular, Caldes de Montbui, 10 march 2018.
3. "*La màgia de l'aigua*". **Toc–Toc UB Science Dissemination Program.**
   Escola Patroncat Domènech, Barcelona, 13 march 2018.
   Biblioteca Sagrada Família, Barcelona, 9 may 2018.
   Escola Patroncat Domènech, Barcelona, 24 october 2018.
   Institut Maria Espinalt, Barcelona, 26 november 2018.
   INS Escola del Treball, Barcelona, 26 november 2018.
4. "*Les microones i les ones de ràdio. Qué són i com ens afecten* ". **Toc–Toc UB Science Dissemination Program.**
   Biblioteca Can Casas, Llinars del Vallès, 8 november 2018.
   Institut Frederic Mompou, Sant Vicenç dels Horts, 14 november 2018.
5. "*La màgia de l'aigua*". **La Setmana de la Ciència.**
   Sala d'Actes UPC, Vilanova i la Geltrú, 13 november 2018.
   La Salle Bonanova, Barcelona, 15 november 2018.
6. "*La màgia de l'aigua*". **Magnet Program, Bofill Foundation.**
   INS La Ribera, Montcada i Reixach, 14 december 2018.
7. *"Podem entendre la Física Quàntica?"* **Feynman birthday, Programa Visions de Ciència.**
   Biblioteca Sagrada Família, Barcelona, 22 january 2018.
8. "*Apropa't a la UB!*"
   Visita de l'Escola Lleó XIII. Universitat de Barcelona, 20 april 2018.
9. *"Feynman i les màquines moleculars: el somni d'un visionari"* **NanoEduca 2018.**
   Universitat de Barcelona, Barcelona, 9 may 2018.

10. *"Poca broma amb la Física Quàntica i Richard Feynman: les contribucions d'un geni"* **Sèrie de conferències i la Setmana de la Ciència 2018.** Agrupació Astronòmica de Sabadell, Sabadell, 14 november 2018.
11. *"Llibres de divulgació científica"* **Màster de Comunicació Científica.** Universitat de Barcelona, Barcelona, 5 november 2018.

Moreover, Prof. Giménez has participated in some interviews in social media:

1. *"Geoingeniaritza, mitoetatik harago"* interviewed by Juanma Gallego. Diari Berria, 28 january 2018. http://www.berria.eus/paperekoa/1974/018/001/2018-01-28/geoingeniaritza_mitoetatik_harago.htm

2. *"Europa obligarà a passar a tots els vehicles matriculats uns tests més exhaustius"*. Interview in "Via Lliure", RAC1, 1 september 2018. https://www.rac1.cat/programes/via-lliure/20180901/451552580540/europa-obligara-a-tots-els-vehicles-matriculats-a-passar-uns-tests-mes-exhaustius.html

3. *"La màgia de l'aigua"*, Toc–Toc UB Programa de disseminació científica, E. Patronat Domènech, Barcelona. 24 october 2018. https://sites.google.com/patronatdomenech.cat/la-mgia-de-laigua/inici

4. *"La màgia de l'aigua"*, Science week 2018. INS Les Vinyes, Cubelles, 15 november 2018. https://agora.xtec.cat/inslesvinyescubelles/general/la-magia-de-laigua/

Here you will find a list of other dissemination activies performed by other IQTC membres during 2018:

1. "*Escalfament global i canvi climàtic*". Francesc Viñes, Escola Can Fabra, 13 june 2018.

2. *"Fem Química al Laboratori"*

   Antonio Aguilar, Jordi Ignés, Carme Sousa and Pablo Gamallo, january-february 2018.

3. *"IV Festa de la Ciència de la UB"*

   Pablo Gamallo, Universitat de Barcelona, 11 may 2018.


*4th Science Party organized by UB*

## II.2 IQTCUB SEMINARS AND CONFERENCES

Dr. Stefan Bromley has continued organizing the seminars and conferences of IQTCUB during 2018. A total of ten seminars and/or conferences, which are listed below:

1. **Dr. Mark Koper** (Leiden University), Leiden, Netherlands.
   *Electrochemistry of Platinum: experiment and theory*
   4 june 2018.

2. **Dr. Sergey Kozlov** (KAUST) Saudi Arabia.
   *Tools to analyse calculated activity of homogeneous and heterogeneous catalysts*
   15 june 2018.

3. **Dr. Kai S. Exner** (University of Sofia), Sofia, Bulgaria.
   *Identifying and closing apparent community gaps in (electro-)chemistry*
   7 november 2018.

4. **Dr. Albert Bruix** (Technical University of Münich), Münich, Germany.
   *Taming the complexity of solid catalysts with the modern modelling toolbox*
   19 december 2018.

5. **Dr. Claudio Narambuena** (Universidad Tecnologica Nacional-CONICET), Argentina.
   *On the reason for α-Lactalbumin adsorption on a charged surface: a study by Monte Carlo simulation*
   12 september 2018.

6. **Prof. Vasil Simeonov** (Universitat de Sofia), Sofia, Bulgaria.
   *The Philosophy of Fake Science*
   29 october 2018.

7. **Prof. Andrey Chuvilin** (CIC nanoGUNE), Donosti, Spain.
   *Electron microscopy lab at CIC nanoGUNE: a guided tour*
   22 june 2018.

## II.3 IQTCUB INVITED RESEARCHERS

During 2018, a total of eigthteen researchers from all over the world have spent some time at the IQTCUB collaborating in different research projects.

1. **Saedeh Kamalinahad** (invited researcher).
   Department of Chemistry, Arak University, Arak, Iran.
   August 2017 - february 2018.

2. **Tomas Lazaukas** (visitor from HPC Europa).
   University College London (UCL), London, UK.
   January 2018.

3. **Prof. Iskra Koleva** (invited researcher).
   Sofia University, Sofia, Bulgaria.
   January-february, july-august 2018.

4. **Prof. Hristiyan Aleksandrov** (invited researcher).
   Sofia University, Sofia, Bulgaria.
   January-february, july-august 2018.

5. **Prof. Nick Brooks** (invited researcher).
   Imperial College London (UCL), London, UK.
   February 2018.

6. **Prof. Sofia Olobardi** (invited researcher).
   Trieste University, Trieste, Italy.
   March-may 2018.

7. **Prof. Galya Madjarova** (invited researcher).
   Sofia University, Sofia, Bulgaria.
   April 2018.

8. **Prof. Petko Petkov** (invited researcher).
   Sofia University, Sofia, Bulgaria.
   May 2018.

9. **Dra. Silvia Acosta** (invited researcher).
   Cagliari University, Cagliari, Italy.
   June-july 2018.

10. **Prof. Jasmina Petrova** (invited researcher).
    Sofia University, Sofia, Bulgaria.
    July 2018.

11. **Dr. Marco Lattuada** (invited researcher).
    University of Fribourg, Friburg, Switzerland.
    July 2018.

12. **Dr. Miroslava Nedyalkova** (Materials Networking European Project).
    Sofia University, Sofia, Bulgaria.
    July-august, october-november 2018.

13. **Prof. Vasil Simeonov** (Materials Networking European Project).
    Sofia University, Sofia, Bulgaria.
    July, october-november 2018.

14. **Dr. Claudio Narambuena** (invited researcher).
    Universidad Tecnologica Nacional-CONICET, Argentina.
    September 2018.

15. **Myriam Torres Rico** (invited researcher).
    University of Sevilla, Sevilla, Spain.
    October-december 2018.

16. **Dr. Kai S. Exner** (invited researcher).
    Sofia University, Sofia, Bulgaria.
    November 2018.

17. **Prof. Jorge Pavez** (invited researcher).
    Universitat de Santiago de Xile, Santiago, Chile.
    November 2018.

18. **Dr. Motoyuki Shiga** (invited researcher).
    Japan Atomic Energy Agency, Japan.
    November 2018.

# III. SCIENTIFIC ACTIVITY OF IQTCUB MEMBERS

## III.1 HIGHLIGHTS FROM MOST RELEVANT RESULTS

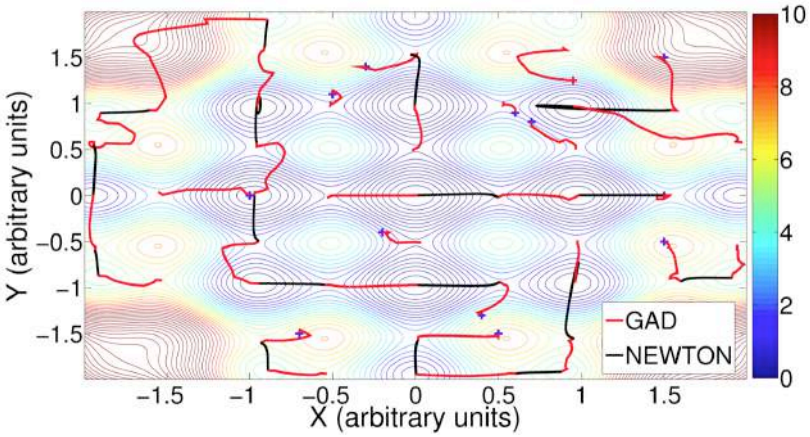
Here some of the most relevant results corresponding to every IQTCUB main research line are presented.

### LINE 1. METHODS, ALGORITHMS AND COMPUTATIONAL TOOLS DEVELOPMENT

**Exploring potential energy surfaces with gentlest ascent dynamics in combination with the shrinking dimer method and Newtonian dynamics.**

G. Albareda, J. M. Bofill, I. De P. R. Moreira, W. Quapp, J. Rubio-Martínez.

**Theor. Chem. Acc.,** *137* (2018) 73.



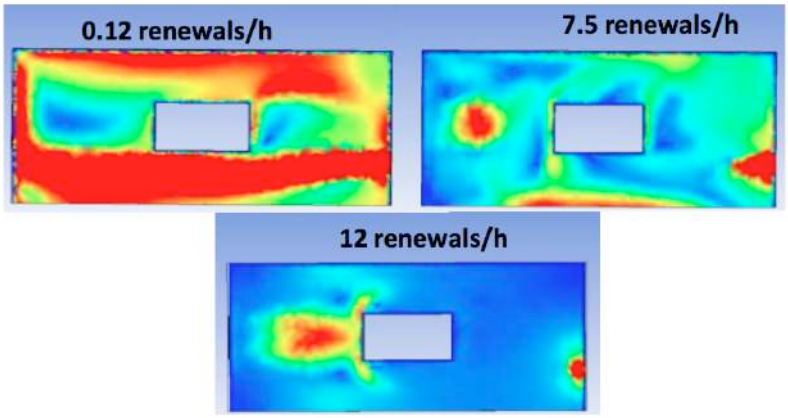

The combination of the proposed method with Newtonian (dissipative) dynamics could lead to a practical scheme for the exhaustive exploration of potential energy landscapes. This is exemplified in the figure for the two-dimensional Rastrigin potential-energy surface, where many possible reaction paths coexist.

In this work, we revisit the so-called gentlest ascent dynamics reaction path model for finding saddle points of any index in multidimensional potential energy surfaces. The variational nature of the method is discussed, and an algorithm for the integration of its equations of motion is proposed. The combination of the proposed method with Newtonian (dissipative) dynamics is proposed as a practical scheme for the exhaustive exploration of potential energy landscapes.

**Immission Assessment Inside an Industrial Ventilated Room Using CFD.**

V. Plesu, A. E. Bonet-Ruiz, J. Bonet, P. Iancu, J. Llorens, L. I. Becerra.

**Chem. Eng. Trans.,** *70* (2018) 1825.




Dependence of the dead zones location on the number of renewals per hour.

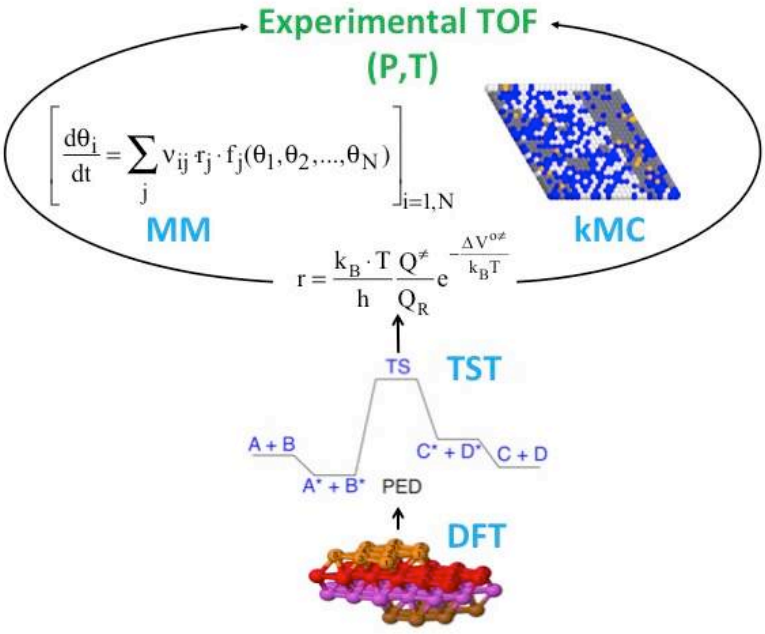
Nowadays the ventilation design of enclosed spaces is based on the number of air renewals per hour. This coarse approach was developed in the past but nowadays is a fast and simple computational exercise to determine where and when the Threshold Limit Value (TLV) is surpassed. A rather superficial Computer Fluid Dynamics (CFD) analysis is able to provide insights that are useful to propose measures to keep the pollutants concentrations at safe levels. The contaminants' level inside a factory is simulated for risk and health assessment to determine the contaminant levels reached as consequence of the normal operation or in case of a sudden release. A good agreement is obtained between simulations and field measurements. A design fulfilling the legislation according to the air renewals tabulated can surpass the TLV in practice. The legislation should be based on CFD results instead of general tabulated values, as in some cases the ventilation could be too oversized or insufficient.

## LINE 2. COMPUTATIONAL MATERIALS SCIENCE

**General concepts, assumptions, drawbacks and misuses in kinetic Monte Carlo and microkinetic modelling simulations applied to computational heterogeneous catalysis**

H. Prats, F. Illas, R. Sayós.

**Int. J. Quantum Chem.,** *118* (2018) e25518.

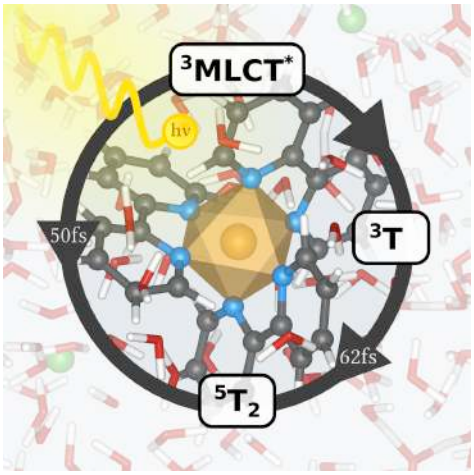



In this article, kinetic Monte Carlo (kMC) and microkinetic models (MM) methods have been reviewed to the study of the heterogeneous catalysis using DFT data. Several important issues that need to be considered for the correct description of complex gas-surface reactions are highlighted. For instance, we provide a quantitative estimate of the effect of neglecting diffusion processes or lateral interactions in kMC simulations. Finally, this paper is expected for serving as a short tutorial for starting researchers in this area.

**Theoretical evidence for the direct $^3$MLCT-HS deactivation in the light-induced spin crossover of Fe(II)–polypyridyl complexes**

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

**Phys. Chem. Chem. Phys.**, *20* (2018) 2351.



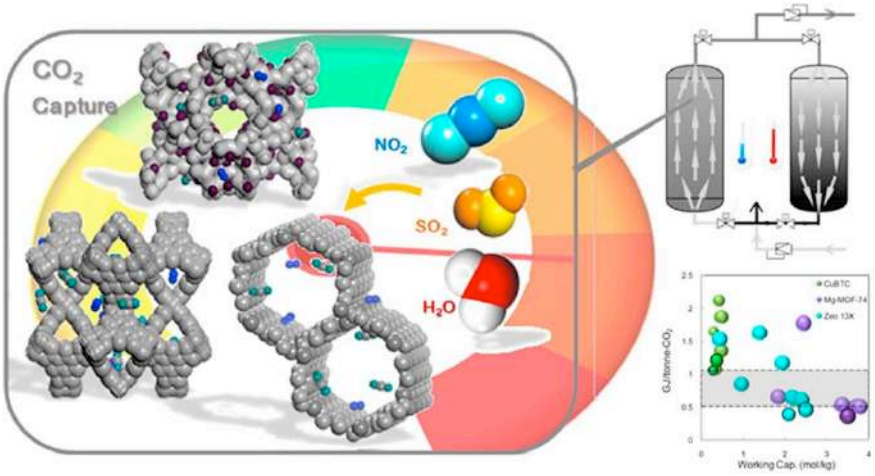

Second-order spin-orbit coupling and structural distorsions activate the $^3$MLCT-$^5T_2$ deactivation in Fe(II)-polypyridyl complexes.

The importance of geometrical distortions and second-order spin-orbit coupling on the intersystem crossing rate constants in the light-induced spin crossover process of the $[Fe(bpy)_3]^{2+}$ complex has been shown. Results prove that a direct channel for the deactivation from the $^3$MLCT state to the final $^5T_2$ state, without intermediate triplet states, is possible when structural disorder is accounted for.

**Energetic evaluation of swing adsorption processes for CO2 capture in selected MOFs and zeolites: effect of impurities**

D. Bahamon, A. Díaz-Márquez, P. Gamallo, L. F. Vega.

**Chem. Eng. J.,** *324* (2018) 458.



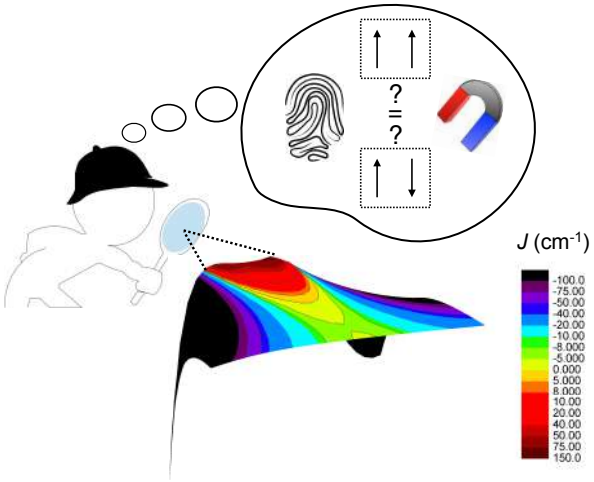

Simulated adsorbent materials and pollutants used in swing adsorption processes.

A systematic computational study of Mg-MOF-74, CuBTC and zeolite 13X for $CO_2$ separation from multicomponent flue gas mixtures is presented. The impurities' impact was evaluated at the molecular level and process conditions. Results show that $NO_2$ has a negligible effect in the studied range. For $H_2O$ and $SO_2$ the energy requirements are reduced as the impurity content increases and recovery and purity increase, up to an optimal point where a competition for $CO_2$ preferred adsorption sites produces a sharp drop in purity and the energetic index grows exponentially.

**The magnetic fingerprint of dithiazolyl-based molecule magnets**

T. Francese, J. Ribas-Arino, J. J. Novoa, R. W. A. Havenith, R. Broer, C. de Graaf, M. Deumal.

**Phys. Chem. Chem. Phys.**, *20* (2018) 20406.




Magnetic bistability in organic-radical based materials has attracted significant interest due to its potential application in electronic devices. In this article, we have presented the results of a first-principles bottom-up study carried out to elucidate the key factors behind the different magnetic response of the low and high temperature phases of four different switchable dithiazolyl (DTA)-based compounds. The change in the magnetic response upon spin transition is always due to the changes in the magnetic interactions between adjacent radicals along the □-stacks of the crystal, which in turn are driven by the changes in the interplanar distance and degree of lateral slippage. Furthermore, specific geometrical dispositions have been recognized as a ferromagnetic fingerprint in such correlations. Our results thus show that an appropriate substitution of the chemical skeleton attached to the DTA ring could give rise to new organic materials with dominant ferromagnetic interactions.

**Properties of hydrated $TiO_2$ and $SiO_2$ nanoclusters: dependence on size, temperature and water vapour pressure**

A. Cuko, A. Macia-Escatllar, M. Calatayud, S. T. Bromley.

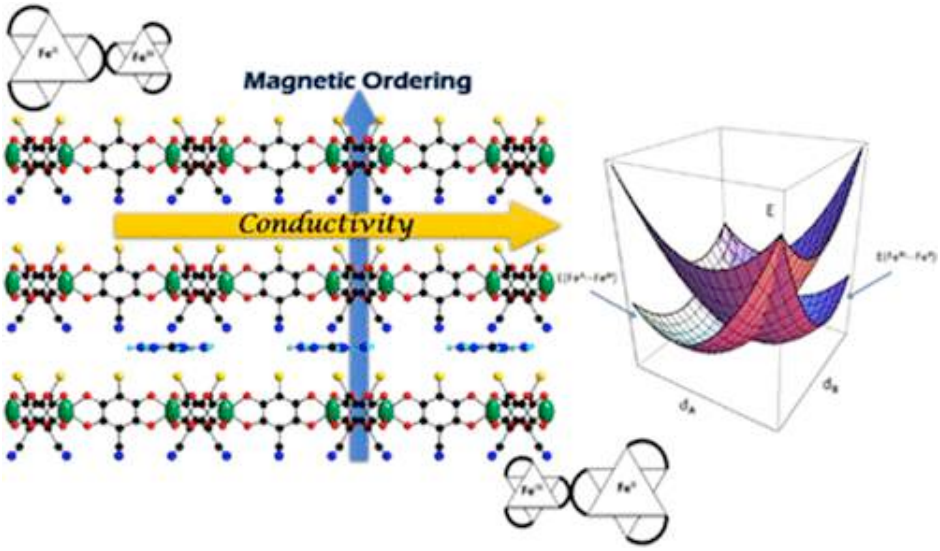
**Nanoscale**, *10* (2018) 21518.

The free energies of titania and silica nanoclusters are accurately modelled with respect to size, temperature, and water vapour pressure.

**Conducting Anilate-Based Mixed-Valence Fe(II)Fe(III) Coordination Polymer: Small-polaron Hopping Model for Oxalate-Type Fe(II)Fe(III) 2D Networks**

S. Sahadevan, A. Abhervé, N. Monni, C. Sáenz de Pipaón, J. R. Galan-Mascaros, J. Waerenborgh, B. Vieira, P. Auban-Senzier, S. Pillet, E. Bendeif, P. Alemany, E. Canadell, M.L. Mercuri, N. Avarvari.

**J. Am. Chem. Soc.**, *140* (2018) 12611-12621.



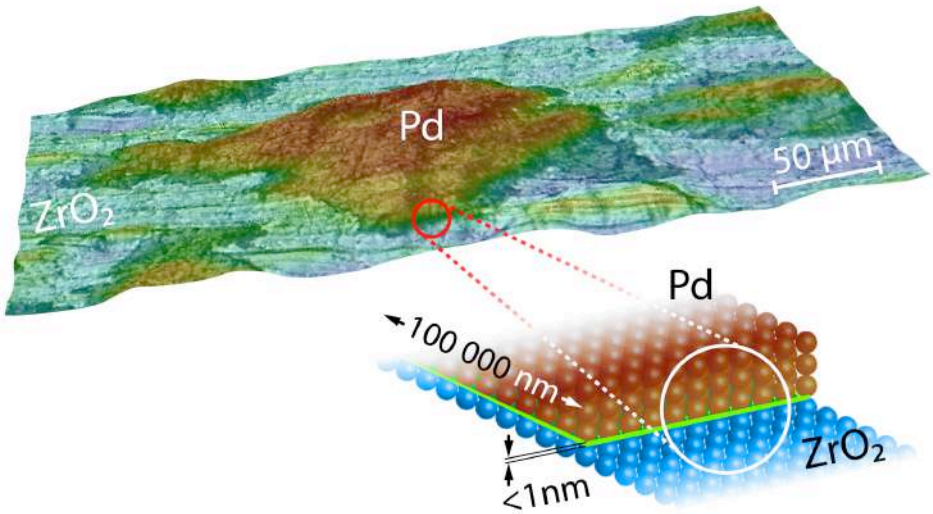

Crystal structure for the coordination polymer highlighting the $Fe^{II}Fe^{III}(anilate)_3$ layers and the directions of electric conductivity and magnetic ordering. The potential energy surface at the right-hand side corresponds to the small-polaron hopping, shown schematically in the top and bottom parts of the figure.

In this work, we report on a multidisciplinar study of the electric and magnetic properties of an interesting coordination polymer formed by iron with the anilate ligand. Our measures show that it is indeed a mixed valence Fe(II)-Fe(III) compound with an unusually high electric conductivity. To answer the question about the origin of this unexpected conductivity we propose a small-polaron hopping model that, in combination with simple quantum chemical calculations for an $Fe(anilate)_3$ monomer, is able to explain why the conductivity should be much higher than in analogous compounds with oxalate or squarate anions.

**The role of metal/oxide interfaces for long-range metal particle activation during CO oxidation**

Y. Suchorski, S. M. Kozlov, I. Bespalov, M. Datler, D. Vogel, Z. Budinska, K. M. Neyman, G. Rupprechter.

**Nature Materials** *17* (2018) 519.



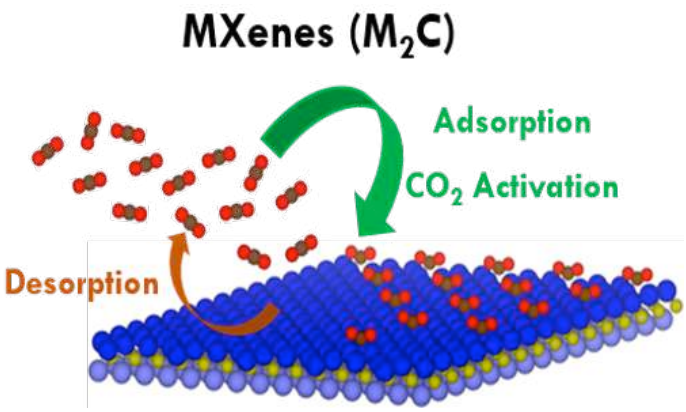

A tiny contact line between Pd grain and support strongly affects CO oxidation on the entire grain that is hundred thousand times larger.

For catalytic particles of thousands of atoms, the support should not affect chemical reactions occurring far away from it. However, an astonishing long-range effect of supports has been visualized, which can make car catalytic converters more efficient for decreasing toxic CO exhaust. Chemical processes on micro-crystallites of palladium catalysts changed significantly, when such particles were supported on inert metal oxides. Namely, the particles remained active for oxidizing CO at higher CO pressure. A very narrow contact line between grains and support influenced CO oxidation over the entire micrometre-size palladium grains. Experiments revealed that catalyst deactivation starts at a grain contacts with the support and from there deactivation spreads like a tsunami wave over the whole grain. These observations are rationalized by calculated stronger binding of oxygen on palladium atoms in direct contact with the support.

**$CO_2$ Abatement Using Two-Dimensional MXene Carbides**

Á. Morales-García, A. Fernández-Fernández, F. Viñes, F. Illas.

**J. Mater. Chem. A.**, *6* (2018) 3381.



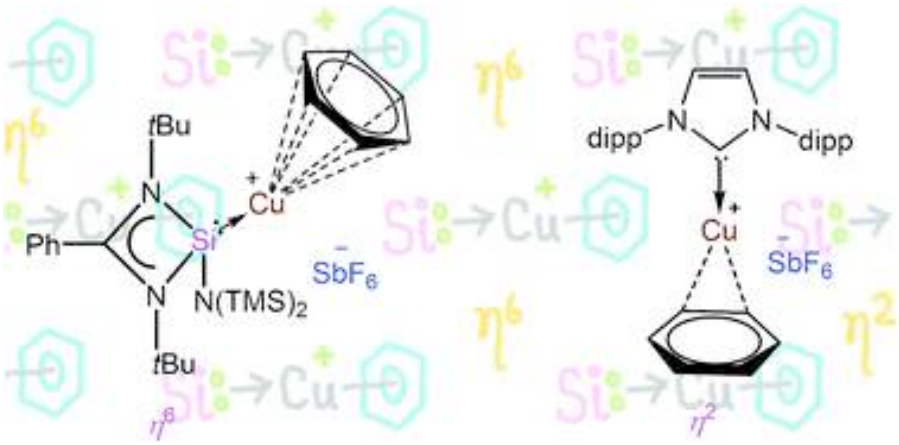

Activation and capture of $CO_2$ on MXene carbides.

The ever-growing concentration of carbon dioxide ($CO_2$) in the atmosphere is one of the major responsible of the greenhouse effect, global warming, and ocean acidification. MXene materials emerge as promising candidates for $CO_2$ chemical anchoring framed within carbon capture and storage (CCS) derived strategies. By means of density functional theory investigations, it has been shown the strong $CO_2$ uptake and activation on carbide MXene with $M_2C$ stoichiometry (M= Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, W), where estimates of adsorption and desorption rates indicate their $CO_2$ adsorption capacity even at low $CO_2$ partial pressures and high temperatures. $M_2C$ materials feature noteworthy $CO_2$ load capacities ranging 2.34-8.25 mol $CO_2$/kg., making MXenes practical materials for $CO_2$ abatement.

**Taming a monomeric Cu($\eta^6$-$C_6H_6$)$^+$ complex with silylene**

N. Parvin, S. Pal, J. Echeverria, S. Alvarez, S. Khan.

**Chem. Sci.**, *9* (2018) 4333-4337.




Different coordination mode of benzene to Cu(I) depending on the additional ligands.

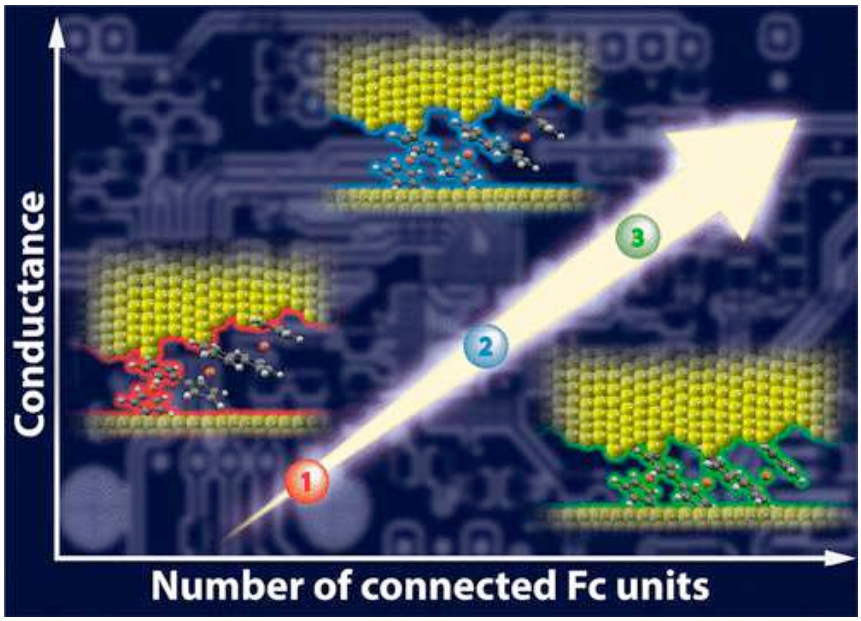
A computational study of a complex with benzene π-coordinated to copper(I) reveals the subtle interplay of steric and electronic factors that favour such a coordination mode in the only compound of that type known so far, synthesized in the group of S. Khan at the Indian Institute of Science Education and Research in Pune. Based on the explanations proposed and on further calculations, predictions of yet unknown compounds that may also showcase that coordination mode between benzene and copper have been made.

## LINE 3. COMPUTATIONAL BIOCHEMISTRY AND *SOFT MATTER*

**Control over Near-Ballistic Electron Transport through Formation of Parallel Pathways in a Single-Molecule Wire**

A. C Aragonès, N. Darwish, S. Ciampi, L. Jiang, R. Roesch, E. Ruiz, C. A Nijhuis, I. Díez-Pérez.

**J. Am. Chem. Soc.**, *141* (2018) 240.

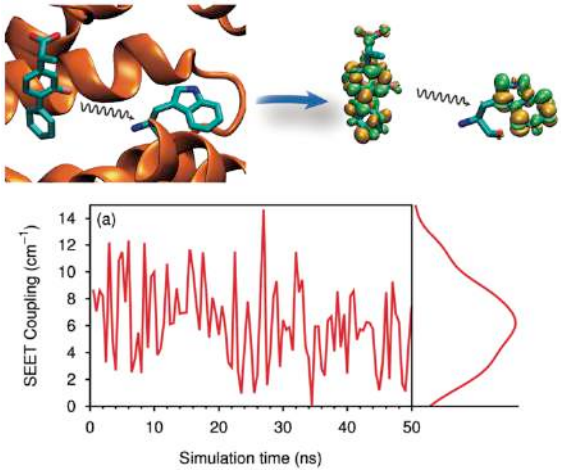



This paper reports highly efficient coherent tunnelling in single-molecules wires of oligo-ferrocenes with one to three Fc units. The Fc units were directly coupled to the electrodes, i.e., without chemical anchoring groups between the Fc units and the terminal electrodes.

**Electronic energy transfer in biomacromolecules**

L. Cupellini, M. Corbella, B. Mennucci, C. Curutchet.

**WIREs Comput. Mol. Sci.**, 2018, in press, doi: 10.1002/wcms.1392.



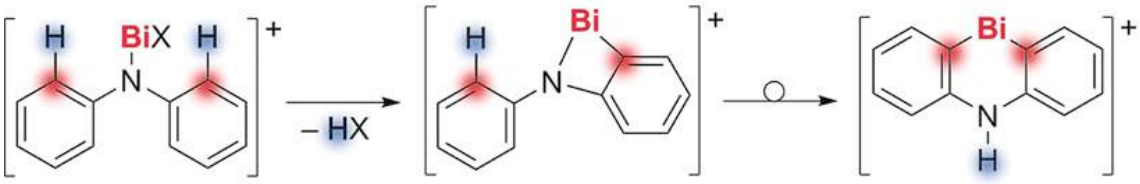

Molecular simulations of energy transfer in biomolecules allow overcoming the main limitations of Förster theory: the point dipole approximation, screening effects, and exciton delocalization.

Electronic energy transfer is widely used as a molecular ruler to interrogate the structure of biomacromolecules, and performs a key task in photosynthesis by transferring collected energy through specialized pigment–protein complexes. Förster theory, introduced over 70 years ago, allows linking transfer rates to simple structural and spectroscopic properties of the energy-transferring molecules. In biosystems, however, significant deviations from Förster behavior often arise due to breakdown of the point dipole approximation, dielectric screening effects due to the biological environment, or departure from the weak-coupling regime. In this review, we provide a concise overview of advances in simulations of energy transfer in biomacromolecules that allow overcoming the main limitations of Förster theory.

**Double CH activation of a masked cationic bismuth amide**

B. Ritschel, J. Poater, H. Dengel, F. M. Bickelhaupt, C. Lichtenberg.

**Angew. Chem. Int. Ed.**, *57* (2018) 3825-3829.

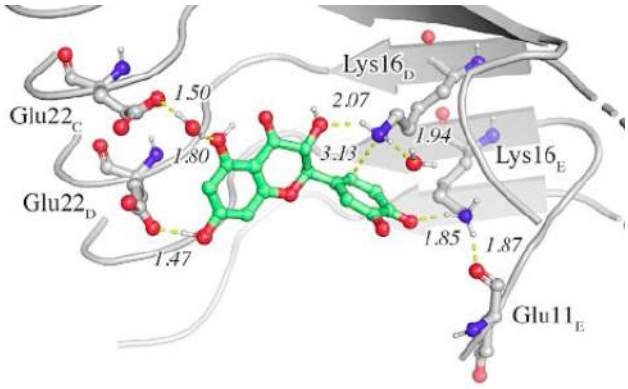



The transformation of C–H bonds into more reactive C–M bonds amenable to further functionalization is of fundamental importance in synthetic chemistry. We demonstrate here that the transformation of neutral bismuth compounds into their cationic analogues can be used as a strategy to facilitate CH activation reactions. In particular, the double CH activation of bismuth-bound diphenyl amide, $(NPh_2)^-$, is reported along with simple one-pot procedures for the functionalization of the activated positions. The organometallic products of the first and second CH activation steps were isolated in high yields. Analysis by NMR spectroscopy, single-crystal X-ray diffraction, and DFT calculations revealed unusual ground-state properties (e.g., ring strain, moderate heteroaromaticity), and provided mechanistic insight into the formation of these compounds.

**Computational Sudy of the Aza-Michael Addition of the Flavonoid (+)-Taxifolin in Inhibition of β-Amyloid Fibril Aggregation**

T. Ginex, M. Trius, F. J. Luque.

**Chem. Eur. J.**, *24* (2018) 5813-5824.



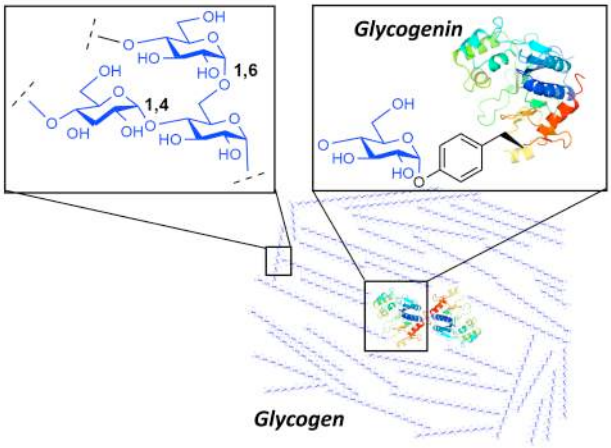

Detail of the binding of (+)-taxifolin to β-amyloid.

The formation of covalent adducts with amyloid fibrils that interfere with the aggregation process opens novel avenues for intervention in amyloidogenic diseases. This study examines the mechanism of formation of a covalent adduct between the oxidized form of (+)-taxifolin and β-amyloid (Aβ42). The results support the involvement of a specific recognition motif that enables the chemical reaction with Aβ42. Thus, (+)-taxifolin binds to the hydrophobic groove delimited by the edges defined by Lys16 and Glu22 residues in the fibril. This mechanism, which may explain the enhanced anti-aggregating activity of oxidized flavonoids, holds promise for developing disease-modifying therapies.

**Palladium-mediated enzyme activation suggests multiphase initiation of glycogenesis**

M. K. Bilyard, H. Bailey, L. Raich, M. Gafitescu, T. Machida, J. Iglesias-Fernández, S. S. Lee, C. D. Spicer, C. Rovira, W. W. Yue, B. G. Davis.

**Nature**, *563* (2018) 235.

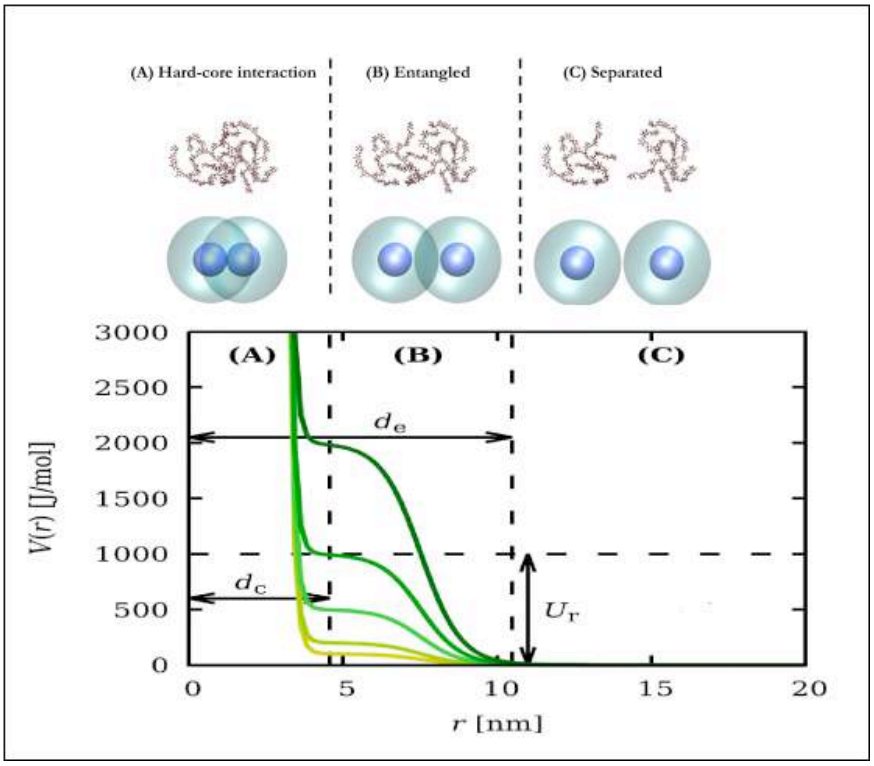



Glycogen is the key energy storage molecule in humans, animals and fungi. It's where the glucose that fuels us is stored and release from. At the heart of the glycogen particle there is a protein that starts the glycogen formation catalysing its own autoglucosylation, that is, decorating itself with glucose molecules. This 'self-sweetening' protein – called glycogenin - has been hard to understand since it acts as both catalyst and substrate, so it is changing continuously during the process. In this work, we have been able to recapitulate and understand mechanistic activity at different stages using a combination of palladium-mediated enzyme activation and molecular dynamics simulations. The results obtained reveal a surprisingly tolerant but precise process to glycogen's creation and growth. The new method used in this work allows to "jump" directly into the intermediate states of glycogening through chemical control and could be a powerful tool in the study of enzymes mechanism.

**Macromolecular diffusion in crowded media beyond the hard-sphere model**

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

**Soft Matter** *14* (2018) 3105-3114.



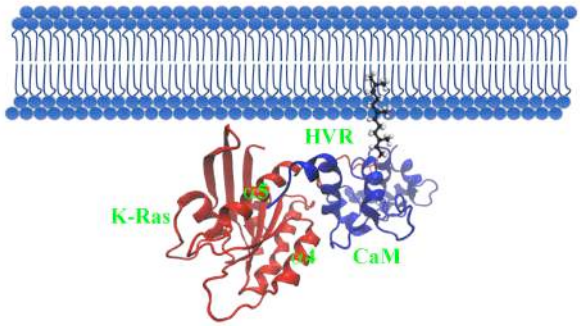

Outline of the Chain Entanglement Soft-Core (CESC) model. Macromolecules are modeled as spheres with two different shells. The outer (transparent) accounts for the interaction between branches and the inner (opaque) accounts for the increasing steric repulsion.

The effect of macromolecular crowding in diffusion beyond the hard-core sphere model is studied. A new soft-core sphere model is presented, the Chain Entanglement Soft Potential (CESP) model, which considers the macromolecular flexibility and chain entanglement. CESP model uses a shoulder-shaped interaction potential which is implemented in the Brownian Dynamics (BD) computations. The interaction potential contains only one parameter associated to the chain entanglement energetic cost ($U_r$). The model is used to analyse the diffusion of streptavidin among different sized dextran obstacles. The obtained long-time diffusion coefficient $D^{long}$ values show better quantitative agreement to experiments than those obtained with hard-core spheres. CESP model is also able to quantitatively predict $D^{long}$ and the anomalous exponent (□) for streptavidin diffusion.

**Modeling and subtleties of K-Ras and Calmodulin interaction**

E. Garrido, J. Lázaro, M. Jaumot, N. Agell, J. Rubio-Martínez.

**PLoS Comput. Biology**, *14* (2018) e1006552.




Proposed model of union of K-Ras with CaM in the presence of plasma membrane.

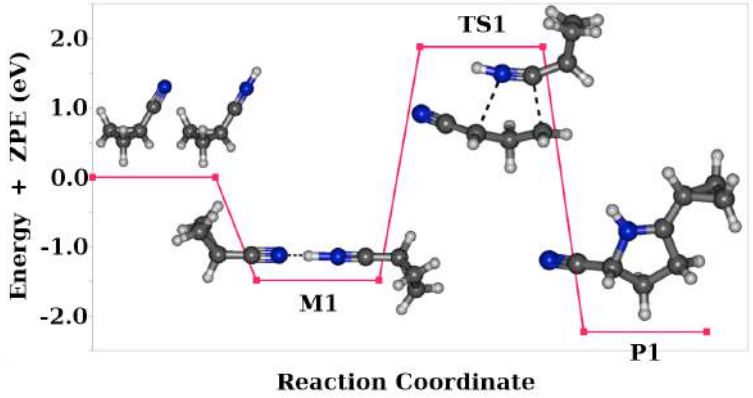
In the present work by using different computational modeling techniques we obtained a model for the K-Ras/Calmoduline interaction that agrees with the experimental data. We believe the present model will help to better understand K-Ras regulation, and to design new inhibitors. For instance, based on our model, we can predict that the interaction can take place at the plasma membrane, and that since the surface of K-Ras that interact with Calmodulin is the same that it uses for dimerization, mimetics of Calmodulin can inhibit K-Ras dimerization.

## LINE 4. REACTIVITY AND REACTIONS DYNAMICS

**The reactivity of the Cyclopropyl cyanide in Titan's atmosphere: a possible pre-biotic mechanism**

E. López, D. Ascenzi, P. Tosi, J. M. Bofill, J. de Andrés, M. Albertí, J. M. Lucas, A. Aguilar.

**Phys. Chem. Chem. Phys.**, *20* (2018) 6198.



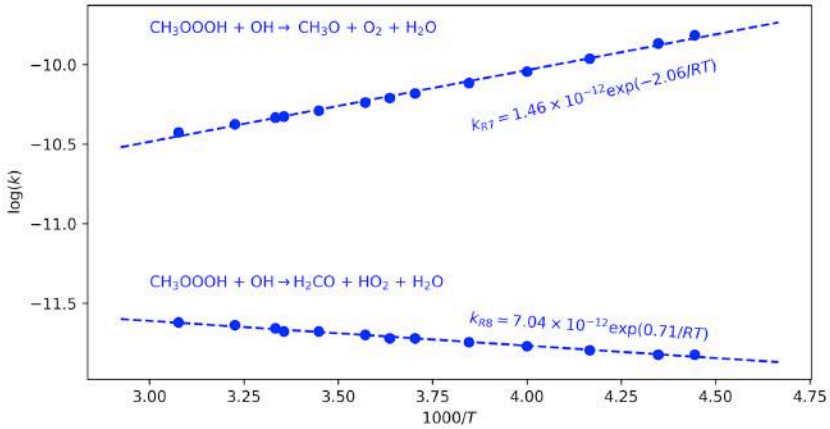

MP2 adiabatic potential energy profile showing the different stationary point (and structures) along the reaction pathway for the $C_4H_5N + C_4H_5NH^+$ reactive process leading to the P1 covalent structure adduct on the ground singlet state of the system.

Cyclopropyl cyanide and other simple nitriles detected on Titan's atmosphere could be precursors leading to the formation of organic macromolecules in its atmosphere. Reaction experiments done between cyclopropyl cyanide and its protonated form, in addition to the expected ion-molecule adduct stabilized by non-covalent long-range interactions, lead to another distinct species having the same mass to charge ratio (*m/z*) of 135 as is proved in this work. From a previous study of the neutral cyclopropyl cyanide potential energy surface (PES) which shows a partial biradical character it has been possible to characterize the formation through the bimolecular reaction of a new covalent cyclic organic molecule at the *ab initio* Möller-Plesset (MP2) level of theory, ensuring the connectivity of the stationary points by using the intrinsic reaction coordinate (IRC) procedure. Characterizing the reaction transition state, multireference calculations were done using a complete active space involving six electrons and six molecular orbitals [CAS (6 $e^-$,6 m.o.)] This study opens the possibility of exploring the formation of new organic molecules by gaseous phase ion-molecule interaction schemes, such molecules having relevance in interstellar space and in astrobiology (and may be involved in the prebiotic molecular evolution).

**Tropospheric oxidation of methyl hydrotrioxide ($CH_3OOOH$) by hydroxyl radical**

J. M. Anglada, A. Solé.

**Phys. Chem. Chem. Phys.**, *20* (2018) 27406-27417.

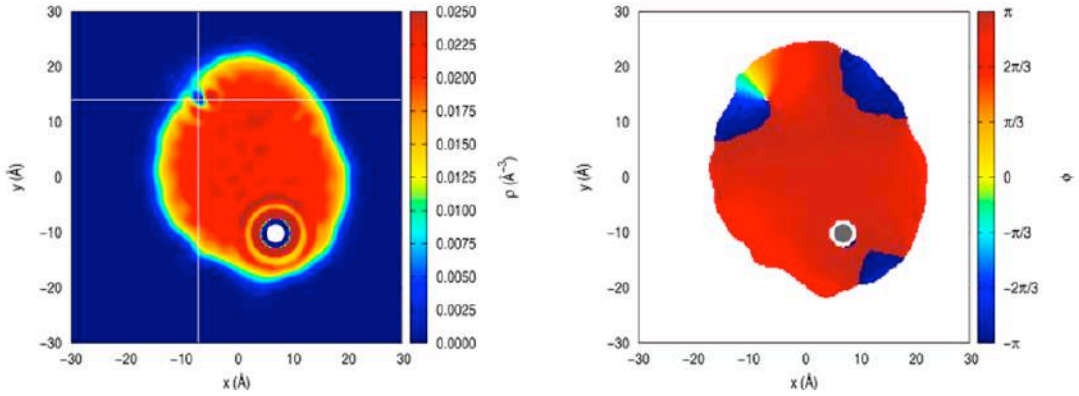



We have employed high level theoretical methods to investigate the oxidation of methyl hydrotrioxide by hydroxyl radical, which is of interest in atmospheric chemistry research. The reaction can proceed by abstraction of either the terminal hydrogen atom of OOH group producing $CH_3O$, $O_2$ and $H_2O$, or one hydrogen atom of the $CH_3$ group forming $H_2CO$, $HO_2$ and $H_2O$. The rate constants for both reactions at 298 K are computed to be $4.7 \times 10^{-11}$ and $2.1 \times 10^{-12}$ $cm^3$ $molecule^{-1}$ $s^{-1}$, respectively, that is, the abstraction of terminal hydrogen atom of the OOH group is about 22 times faster than that of a hydrogen atom of the $CH_3$ group. The rate constant for the overall $CH_3OOOH$ + OH reaction is computed to be $4.9 \times 10^{-11}$ $cm^3$ $molecule^{-1}$ $s^{-1}$. Our calculations predict branching ratios between 99.0 and 93.9% for the formation of methoxy radical plus molecular oxygen and water, and between 1.0 and 6.1% for the formation of formaldehyde plus hydroperoxyl radical and water, in the 225–325 K temperature range. The lifetime of $CH_3OOOH$ in the troposphere is predicted to range from of 1.8 hours at 225 K, up to 3.9 hours at 275 K and decreasing to 0.2 hours at 310 K.

**Quantum-classical dynamics of the capture of neon atoms by superfluid helium nanodroplets**

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

**Phys. Chem. Chem. Phys.**, *20* (2018) 29737.




Quantized vortex in the top left part of the helium density (left) and phase of the helium wave function (right), for the most probable velocity of Ne at 300 K ($v_0$=500 m s$^{-1}$), impact parameter $b$=17 Å and final simulation time (171.2 ps).

The capture of a Ne atom by a superfluid helium nanodroplet, Ne + $(^4He)_N$ → Ne@$(^4He)^{N'}$ + (N-N') $^4$He, was studied using a hybrid quantum (helium)-classical (Ne) approach, taking into account for the first time the angular momentum (and the resulting vortex formation) in a detailed way. Large energy and angular momentum transfer from the atom to the nanodroplet occur and the angular momentum of the Ne atom can induce vortex nucleation for high enough initial angular momentum values (~176.3-220.3 $\hbar$). Vortices arise from collapse of the surface excitations (ripplons) and are long-lived for some initial conditions. Comparison with a previous quantum dynamics study of our own at zero angular momentum shows that quantum effects are not important under the initial conditions examined here. Besides, a comparison with the scarce information available on other systems has been performed, showing the rich variety of behaviours that can be observed in the solvation of impurities by superfluid helium.

## III.2 PUBLICATION LIST

### PUBLISHED ARTICLES

1. *Biogas upgrading by transition metal carbides.*
C. Kunkel, F. Viñes, F. Illas.
**ACS Appl. Energy Mater.** *1* (2018) 43-47.

2. *Alkali metal cation effects in structuring Pt, Rh, and Au surfaces through cathodic corrosion.*
T. J. P. Hersbach, I. T. McCrum, D. Anastasiadou, R. Wever, F. Calle-Vallejo, M. T. M. Koper**.**
**ACS Appl. Mater. Interfaces** *10* (2018) 39363-39379.

3. *QM/MM studies into the $H_2O_2$-dependent activity of lytic polysaccharide monooxygenases: evidence for the formation of a caged hydroxyl radical intermediate.*
B. Wang, E. M. Johnston, P. Li, S. Shaik, G. J. Davies, P. H. Walton, C. Rovira.
**ACS Catal.** *8* (2018) 346–1351.

4. *Can an alcohol act as an acid/base catalyst in water solution? An experimental and theoretical study of imidazole catalysis of the aqueous Morita–Baylis–Hillman reaction.*
L. Raich, H. Santos, J. C Gomes, M. T. Rodrigues, R. Galaverna, M. N. Eberlin, F. Coelho, C. Rovira, A. Moyano.
**ACS Catal.** *8* (2018) 1703–1714. editorially selected as *Hot Paper.*

5. *Structural and mechanistic insights into the catalytic domain-mediated short-range glycosylation preferences of GalNAc-T4.*
M. de las Rivas, E. J. P. Daniel, H. Coelho, E. Lira-Navarrete, L. Raich, I. Compañón, A. Diniz, L. Lagartera, J. Jiménez-Barbero, H. Clausen, C. Rovira, F. Marcelo, F. Corzana, T. A. Gerken, R. Hurtado-Guerrero.
**ACS Centr. Sci.** *4* (2018) 1274-1290.

6. *The molecular mechanism of substrate recognition and catalysis of the membrane acyltransferase PatA from mycobacteria.*
M. Tersa, L. Raich, D. Albesa-Jové, B. Trastoy, J. Prandi, M. Gilleron, C. Rovira, M. E. Guerin.
**ACS Chem. Biol.** *13* (2018) 131-140.

7. *Computational comparison of late transition metal (100) surfaces for the electrocatalytic reduction of CO to $C_2$ species.*
S. Hanselman, M. T. M. Koper, F. Calle-Vallejo**.**
**ACS Energy Lett.** *3* (2018) 1062-1067.

8. *An unprecedented stimuli-controlled single-crystal reversible phase transition of a metal-organic framework and its application to a novel method of guest encapsulation.*
F. C. Tan, A. López-Periago, M. E. Light, J. Cirera, E. Ruiz, A. Borras, F. Teixidor, C. Viñas, C. Domingo, J. G. Planas.
**Adv. Mater.** *30* (2018) 1800726.

9. *Double CH activation of a masked cationic bismuth amide.*
B. Ritschel, J. Poater, H. Dengel, F. M. Bickelhaupt, C. Lichtenberg
**Angew. Chem. Int. Ed.** *57* (2018) 3825-3829.

10. *Subsurface carbon: a general feature of noble metals.*
O. Piqué, I. Koleva, F. Viñes, H. Aleksandrov, G. N. Vayssilov, F. Illas.
**Angew. Chem. Int. Ed.** doi: 10.1002/anie.201813037

11. *Recognition of shorter and longer trimethyllysine analogues by epigenetic reader proteins.*
A. H. K. Al Temimi, R. Belle, K. Kumar, J. Poater, P. Betlem, B. J. G. E. Pieters, R. S. Paton, F. M. Bickelhaupt, J. Mecinovic.
**Chem. Comm.** *54* (2018) 2409-2412.

12. *Energetic evaluation of swing adsorption processes for $CO_2$ capture in selected MOFs and zeolites: effect of impurities.*
D. Bahamon, A. Díaz-Márquez, P. Gamallo, L. F. Vega.
**Chem. Eng. J.** *342* (2018) 458-473.

13. *Immission Assessment Inside an Industrial Ventilated Room Using CFD.*
V. Plesu, A. E. Bonet-Ruiz, J. Bonet, P. Iancu, J. Llorens, L. I. Becerra.
**Chem. Eng. Trans.** *70* (2018) 1825-1830.

14. *Surrogate Model for Carbon Dioxide Equilibrium Absorption Using Aqueous Monoethanolamine.*
V. Plesu, J. Bonet, A.E. Bonet-Ruiz, A. Chavarria, P. Iancu, J. Llorens.
**Chem. Eng. Trans.** *70* (2018) 919-924.

15. *A heuristic for extractive agent flow rate in extractive distillation.*
V. Plesu, S. Cantero, A. E. Bonet-Ruiz, J. Bonet, P. Iancu, J. Llorens.
**Chem. Eng. Trans.** *70* (2018) 1849-1854.

16. *Effect of second-order spin-orbit coupling on the interaction between spin states in spin-crossover systems.*
C. Sousa, A. Domingo, C. de Graaf.
**Chem. Eur. J.** *24* (2018) 5146-5152.

17. *Theory uncovers the role of the methionine–tyrosine–tryptophan radical adduct in the catalase reaction of KatGs: $O_2$ release mediated by proton-coupled electron transfer.*
B. Wang, I. Fita, C. Rovira.
**Chem. Eur. J.** *24* (2018) 5388-5395.

18. *Computational sudy of the aza-Michael addition of the flavonoid (+)-taxifolin in inhibition of β-amyloid fibril aggregation.*
T. Ginex, M. Trius, F. J. Luque.
**Chem. Eur. J.** *24* (2018) 5813-5824.

19. *A pseudo-octahedral Cobalt(II) complex with bispyrazolylpyridine ligands acting as a zero-field single-molecule magnet with easy axis anisotropy.*
L. Rigamonti, N. Bridonneau, G. Poneti, L. Tesi, L. Sorace, D. Pinkowicz, J. Jover, E. Ruiz, R. Sessoli, A. Cornia.
**Chem. Eur. J.** *24* (2018) 8857-8868.

20. *Boosting self-assembly diversity in the solid-state by chiral/non-chiral $Zn^{II}$-porphyrin crystallization.*
W. J. Qian, A. González-Campo, A. Pérez-Rodríguez, S. Rodríguez-Hermida, I. Imaz, K. Wurst, D. Maspoch, E. Ruiz, C. Ocal, E. Barrena, D. B. Amabilino, N. Aliaga-Alcalde.
**Chem. Eur. J.** *24* (2018) 12950-12960.

21. *Multiple multicomponent reactions: unexplored substrates, selective processes and versatile chemotypes in biomedicine.*
O. Ghashghaei, S. Caputo, M. Sintes, M. Revés, N. Kielland, C. Estarellas, F. J. Luque, A. Aviñó, R. Eritja, A. Serna-Gallego, J. A. Marrugal-Lorenzo, J. Pachón, J. Sánchez-Céspedes, R. Treadwell, F. de Moliner, M. Vendrell, R. Lavilla.
**Chem. Eur. J.** *24* (2018) 14513-14521.

22. *Oxazoline or oxazolinium ion? the protonation state and conformation of the reaction intermediate of chitinase enzymes revisited.*
J. Coines, M. Alfonso-Prieto, X. Biarnés, A. Planas, C. Rovira.
**Chem. Eur. J.** *24* (2018) 19258-19265.

23. *Deactivation of excited states in transition□metal complexes: insight from computational chemistry.*
C. Sousa, M. Alías, A. Domingo, C. de Graaf.
**Chem. Eur. J.** (2018) doi: 10.1002/chem.201801990.

24. *Mechanical tuning of through-molecule conductance in a conjugated calix [4] pyrrole.*
D. Stefani, M. Perrin, C. Gutiérrez-Cerón, A. C. Aragonès, J. Labra-Muñoz, R. D. C. Carrasco, Y. Matsushita, Z. Futera, J. Labuta, T. H. Ngo, K. Ariga, I. Díez-Pérez, H. S. J. van der Zant, D. Dulić, J. P. Hill.
**ChemistrySelect** *3* (2018) 6473-6478.

25. *A global optimisation study of the low-lying isomers of the alumina octomer $(Al_2O_3)_8$.*
D. Gobrecht, L. Decin, S. Cristallo, S. T.Bromley.
**Chem. Phys. Lett.** *711* (2018) 138-147.

26. *Taming a monomeric $Cu(\eta^6\text{-}C_6H_6)^+$ complex with silylene.*
N. Parvin, S. Pal, J. Echeverria, S. Alvarez, S. Khan.
**Chem. Sci.** *9* (2018) 4333-4337.

27. *Electric-field induced bistability in single-molecule conductance measurements for boron coordinated curcuminoid compounds.*
I. J. Olavarria-Contreras, A. Etcheverry-Berrios, W. J. Qian, C. Gutierrez-Ceron, A. Campos-Olguin, E. C. Sanudo, D. Dulic, E. Ruiz, N. Aliaga-Alcalde, M. Soler, H. S. J. van der Zant.
**Chem. Sci.** *9* (2018) 6988-6996.

28. *Harnessing electrostatic catalysis in single molecule, electrochemical and chemical systems: a rapidly growing experimental tool box.*
S. Ciampi, N. Darwish, H. M. Aitken, I. Díez-Pérez, M. L. Coote.
**Chem. Soc. Rev.** *47* (2018) 5146-5164.

29. *Enabling generalized coordination numbers to describe strain effects.*
F. Calle-Vallejo, A. S. Bandarenka.
**ChemSusChem** *11* (2018) 1824-1828.

30. *Two-dimensional silicon carbide structure under uniaxial strains, electronic and bonding analysis.*
S. Belarouci, T. Ouahrani, N. Benabdallah, Á. Morales-García, I. Belabbas.
**Comput. Mater. Sci.** 151 (2018) 288-295.

31. *$(BEDT\text{-}TTF)_2Cu_2(CN)_3$ spin líquid: beyong the average structure.*
P. Foury-Leylekian, V. Ilakovac, V. Balédent, P. Fertey, A. Arakcheeva, O. Milat, D. Petermann, G. Guillier, K. Miyagawa, K. Kanoda, P. Alemany, E. Canadell, S. Tomic, J. P. Pouget.
**Crystals** *8* (2018) 158.

32. *Indirect effect of hydrogen bonds on the magnetic coupling on Mn(III) dinuclear compounds.*
J. M. Pagès, L. Escriche-Tur, M. Font-Bardia, G. Aullón, M. Corbella.
**Cryst. Eng. Comm.** *20* (2018) 6629-6639.

33. *Noncovalent interactions in succinic and maleic anhydride derivatives.*
J. Echeverria.
**Cryst. Growth Des.** *18* (2018) 506-512.

34. *Does the breaking of adsorption-energy scaling relations guarantee enhanced electrocatalysis?*
N. Govindarajan, J. M. García-Lastra, E. J. Meijer, F. Calle-Vallejo.
**Curr. Opin. Electrochem.** *8* (2018) 110-117.

35. *A brief review of the computational modeling of $CO_2$ electroreduction on Cu electrodes.*
A. Rendón-Calle, S. Builes, F. Calle-Vallejo.
**Curr. Opin. Electrochem.** *9* (2018) 158-165.

36. *Slow relaxation of magnetization in a bis-mer-tridentate octahedral Co(II) complex.*
D. Sertphon, K. S. Murray, W. Phonsri, J. Jover, E. Ruiz, S. G. Telfer, A. Alkas, P. Harding, D. J. Harding.
**Dalton Trans.** *47* (2018) 859-867.

37. *A 2D rhomboidal system of Mn(II) [Mn(3-MeC$_6$H$_4$COO)$_2$(H$_2$O)$_2$]$_n$ with spin canting: rationalization of the magnetic exchange.*
B. García-Cirera, R. Costa, I. De P. R. Moreira, M. Font-Bardia, M. Corbella.
**Dalton Trans.** *47* (2018) 3717-3724.

38. *Evaluation of novel platinum(II) based AIE compound-encapsulated mesoporous silica nanoparticles for cancer theranostic application.*
S. Saleem Pasha, L. Fageria, C. Climent, N. P. Rath, P. Alemany, R. Chowdhury, A. Roy, I. R. Laskar.
**Dalton Trans.** *47* (2018) 4613-4624.

39. *Easily reduced bis-pincer (NS$_2$)$_2$molybdenum(IV) to (NHS$_2$)$_2$Mo(II) by alcohols vs. redox-inert (NS$_2$)(NHS$_2$)iron(III) complexes.*
E. Robles-Marin, A. Mondragón, P. R. Martínez-Alanis, G. Aullón, M. Flores-Alamo, I. Castillo.
**Dalton Trans.** *47* (2018) 10932-10940.

40. *Pre-selection and assessment of green organic solvents by clustering chemometric tools.*
M. Tobiszewski, M. Nedyalkova, S. Madurga, F. Pena-Pereira, J. Namie□nik, V. Simeonov.
**Ecotox. Environ. Safe.** *147* (2018) 292-298.

41. *Interconversions of nitrogen-containing species on Pt(100) and Pt(111) electrodes in acidic solutions containing nitrate.*
I. Katsounaros, M. C. Figueiredo, X. Chen, F. Calle-Vallejo, M. T. M. Koper**.**
**Electrochim. Acta.** *271* (2018) 77-83.

42. *H-mediated magnetic interactions between layers in a 2D Mn$^{II}$-dicyanamide polymer: neutron diffraction, DFT, and quantum Monte Carlo calculations.*
B. Gillon, A. Hammerschmied, A. Gukasov, A. Cousson, T. Cauchy, E. Ruiz, J. A. Schlueter, J. L. Manson.
**Eur. J. Inorg. Chem.** (2018) 278-288.

43. *Antiferromagnetic interactions in Copper(II) $\mu$-oxalato dinuclear complexes: the role of the counterion.*
M. Julve, A. Gleizes, L. M. Chamoreau, E. Ruiz, M. Verdaguer.
**Eur. J. Inorg. Chem.** (2018) 509-516.

44. *Substituted tetrahydroisoquinolines: synthesis, characterization, antitumor activity and other biological properties.*
S. Capilla, R. Soucek, L. Grau, M. Romero, J. Rubio-Martínez, D. H. Caignard, M. D. Pujol.
**Eur. J. Med. Chem.** *145* (2018) 51-63.

45. *First homology model of plasmodium falciparum glucose-6-phosphate dehydrogenase: discovery of selective substrate analog-based inhibitors as novel antimalarial agents.*
N. Alencar, I. Sola, M. Linares, J. Juárez-Jiménez, C. Pont, A. Viayna, D. Vílchez, C. Sampedro, P. Abad, S. Pérez-Benavente, J. Lameira, J. M. Bautista, D. Muñoz-Torrero, F. J. Luque.
**Eur. J. Med. Chem.** *146* (2018) 108-122.

46. *Aromaticity determines the relative stability of kinked vs. straight topologies in polycyclic aromatic hydrocarbons.*
J. Poater, M. Duran, M. Solà.
**Front. Chem.** *6* (2018) 561.

47. *A multistep docking and scoring protocol for congeneric series: implementation on kinase DFG-out type II inhibidors.*
J. M. Granadino-Roldán, A. Garzón, P. Gomez-Gutierrez, I. Pasamontes-Funez, M. S.Tomas, J. Rubio-Martinez.
**Future Med. Chem.** *10* (2018) 297-318.

48. *Electronic and steric control of the spin-crossover behavior in $(Cp^R)_2Mn$ manganocenes.*
J. Cirera, E. Ruiz.
**Inorg. Chem.** *57* (2018) 702-709.

49. *Designing a $Dy_2$ single-molecule magnet with two well differentiated relaxation processes by using a nonsymmetric bisbidentate bipyrimidine-N-oxide ligand: a comparison with mononuclear counterparts.*
F. Diaz-Ortega, J. M. Herrera, D. Aravena, E. Ruiz, T. Gupta, G. Rajaraman, H. Nojiri, E. Colacio.
**Inorg. Chem.** *57* (2018) 6362-6375.

50. *Effect of heteroatoms on field-induced slow magnetic relaxation of mononuclear $Fe^{III}$ (S=5/2) Ions within polyoxometalates.*
T. Minato, D. Aravena, E. Ruiz, K. Yamaguchi, N. Mizuno, K. Suzuki.
**Inorg. Chem.** *57* (2018) 6957-6964.

51. *Covalent and ionic capacity of MOFs to sorb small gas molecules.*
J. Poater, M. Gimferrer, A. Poater.
**Inorg. Chem.** *57* (2018) 6981-6990.

52. *Kineticomechanistic study of the redox pH cycling processes occurring on a robust water-soluble cyanido-bridged mixed-valence {$Co^{III}/Fe^{II}$}$_2$ square.*
L. Alcázar, P. V. Bernhardt, M. Ferrer, M. Font-Bardia, A. Gallen, J. Jover, M. Martínez, J. Peters, T. J. Zerk.
**Inorg. Chem.** *57* (2018) 8465-8475.

53. *Element-selective molecular charge transport characteristics of binuclear copper(II)-lanthanide(III) complexes.*
S. Schmitz, A. Kovalchuk, A. Martín-Rodríguez, J. van Leusen, N. V. Izarova, S. D. M. Bourone, Y. Ai, E. Ruiz, R. C. Chiechi, P. Kogerler, K. Y. Monakhov.
**Inorg. Chem.** *57* (2018) 9274-9285.

54. *Mononuclear lanthanide complexes with 18-crown-6 ether: synthesis, characterization, magnetic properties, and theoretical studies.*
L. Maxwell, M. Amoza, E. Ruiz.
**Inorg. Chem.** *57* (2018) 13225-13234.

55. *Benchmarking density functional methods for calculation of state energies of first row spin-crossover molecules.*
J. Cirera, M. Via-Nadal, E. Ruiz.
**Inorg. Chem.** *57* (2018) 14097-14105.

56. *Zero- and mono-coordinate transition metals in crystal structures: a box full of surprises.*
S. Alvarez.
**Inorg. Chim. Acta** *470* (2018) 74-81.

57. *General concepts, assumptions, drawbacks and misuses in kinetic Monte Carlo and microkinetic modelling simulations applied to computational heterogeneous catalysis.*
H. Prats, F. Illas, R. Sayós.
**Int. J. Quantum Chem.** *118* (2018) e25518.

58. Mechanochemistry on the Müller-Brown surface.
W. Quapp, J. M. Bofill
**Int. J. Quantum Chem.** *118* (2018) e25522.

59. *Toward a theory of mechanochemistry: simple models from the very beginnings.*
W. Quapp, J.M. Bofill, J. Ribas-Arino.
**Int. J. Quantum Chem.** 118 (2018) e25775.

60. *Three-body molecular states of the $LiH_2^+$ system in the Born-Oppenheimer approximation.*
E. J. Randazzo, A. Aguilar-Navarro.
**Int. J. Quantum Chem.** *118* (2018) e25611.

61. *Control over near-ballistic electron transport through formation of parallel pathways in a single-molecule wire.*
A. C Aragonès, N. Darwish, S. Ciampi, L. Jiang, R. Roesch, E. Ruiz, C. A. Nijhuis, I. Díez-Pérez.
**J. Am. Chem. Soc.** *141* (2018) 240-250.

62. *Conducting anilate-based mixed-vpero alence Fe(II)Fe(III) coordination polymer: small-polaron hopping model for oxalate-type Fe(II)Fe(III) 2D networks.*
S. Sahadevan, A. Abhervé, N. Monni, C. Sáenz de Pipaón, J. R. Galan-Mascaros, J. Waerenborgh, B. Vieira, P. Auban-Senzier, S. Pillet, E. Bendeif, P. Alemany, E. Canadell, M.L. Mercuri, N. Avarvari.
**J. Am. Chem. Soc.** *140* (2018) 12611-12621.

63. *Molecular-scale ligand effects in small gold-thiolate nanoclusters.*
D. M. Chevrier, L. Raich, C. Rovira, A. Das, Z. Luo, Q. Yao, A. Chatt, J. Xie, R. Jin, J. Akola, P. Zhang.
**J. Am. Chem. Soc.** *140* (2018) 15430-15436.

64. *On the mechanism of the electrochemical conversion of ammonia to dinitrogen on Pt(100) in alkaline environment.*
I. Katsounaros, M. C. Figueiredo, X. Chen, F. Calle-Vallejo, H. Li, A. A. Gewirth, N. M. Markovic, M. T. M. Koper**.**
**J. Catal.** *359* (2018) 82-91.

65. *Thermal stability of globins: implications of flexibility and heme coordination studied by molecular dynamics simulations.*
L. Julió Plana, A. Nadra, D. Estrin, F. J. Luque, L. Capece.
**J. Chem. Inf. Model.** *59* (2018) 441-452.

66. *Development and validation of molecular overlays derived from 3D hydrophobic similarity with PharmScreen.*
J. Vázquez, A. Deplano, A. Herrero, T. Ginex, E. Gibert, O. Rabal, J. Oyarzabal, E. Herrero, F. J. Luque.
**J. Chem. Inf. Model.** *24* (2018) 1596-1609.

67. *Jacob's ladder as sketched by Escher: assessing the performance of broadly-used density functionals on transition metal surface properties.*
L. Vega, J. Ruvireta, F. Viñes, F. Illas.
**J. Chem. Theory Comput.** *14* (2018) 395-403.

68. *Assessing GW approaches for predicting core level binding energies.*
M. J. Van Setten, R. Costa, F. Viñes, F. Illas.
**J. Chem. Theory Comput.,** *14* (2018) 877-883.

69. *Density-dependent formulation of dispersion−repulsion interactions in hybrid multiscale quantum/molecular mechanics (QM/MM) models.*
C. Curutchet, L. Cupellini, J. Kongsted, S. Corni, L. Frediani, A. H. Steindal, C. A. Guido, G. Scalmani, B. Mennucci.
**J. Chem. Theory Comput.** *14* (2018) 1671-1681.

70. *Theoretical modeling of electronic excitations of gas-phase and solvated $TiO_2$ nanoclusters and nanoparticles of interest in photocatalysis.*
R. Valero, Á. Morales-García, F. Illas.
**J. Chem. Theory Comput.** *14* (2018) 4391-4404.

71. *Electronic and structural properties of $Li_n@Be_2B_8$ (n=1-14) and $Li_n@Be_2B_{36}$ (n=1-21) nanoflakes shed light on possible anode materials for Li based batteries.*
M. Goodarzi, F. Nazari, F. Illas.
**J. Comput. Chem.** *39* (2018) 1795-1805.

72. *Rational* design of near-infrared absorbing organic dyes: controlling the HOMO-LUMO gap using quantitative molecular orbital theory.
A. K. Narsaria, J. Poater, C. Fonseca-Guerra, A. W. Ehlers, K. Lammertsma, F. M. Bickelhaupt.
**J. Comput. Chem.** *39* (2018) 2690-2696.

73. *Shapes of undecanuclear clusters and undecacoordinated metal complexes.*
S. Alvarez.
**J. Coord. Chem.** *71* (2018) 590-600.

74. *$CO_2$ abatement by two-dimensional MXene carbides.*
Á. Morales-García, A. Fernández-Fernández, F. Viñes, F. Illas.
**J. Mater. Chem. A** *6* (2018) 3381-3385.

75. *Pressure-induced chemistry for the 2D to 3D transformation of zeolites.*
M. Mazur, Á. M. Arévalo-López, P. S. Wheatley, G. P. Bignami, S. E. Ashbrook, Á. Morales-García, P. Nachtigall, J. P. Attfield, J. Cejka, R. E. Morris.
**J. Mater. Chem. A** *6* (2018) 5255-5259.

76. *Visible and near-infrared organic photosensitizers comprising isoindigo derivatives as chromophores: synthesis, optoelectronic properties and factors limiting their efficiency in dye solar cells.*
C. Aumaitre, C. Rodríguez-Seco, J. Jover, O. Bardagot, F. Caffy, Y. Kervella, N. López, E. Palomares, R. Demadrille.
**J. Mater. Chem. A** *6* (2018) 10074-10084.

77. *Influence of texture on the electrical properties of Al-doped ZnO films prepared by ultrasonic spray pyrolysis.*
J. A. Barón-Miranda, O. Calzadilla, S. San-Juan-Hernández, I. Diez-Pérez, J. Díaz, F. Sanz, F. F. Chále-Lara, F. J. Espinosa-Faller, F. Caballero-Briones.
**J. Mater. Sci-Mater. El.** *29* (2018) 2016-2025.

78. *Aniline-based inhibitors of influenza H1N1 virus acting on hemagglutinin-mediated fusion.*
R. Leiva, M. Barniol-Xicota, S. Codony, T. Ginex, E. Vanderlinden, M. Montes, M. Caffrey, F. J. Luque, L. Naesens, S. Vázquez.
**J. Med. Chem.** *61* (2018) 98-118.

79. *Redesigning the coumarin scaffold into small bright fluorophores with far-red to NIR emission and large Stokes' shifts useful for cell imaging.*
A. Gandioso, R. Bresolí-Obach, A. Nin-Hill, M. Bosch, M. Palau, A. Galindo, S. Contreras, C. Rovira, S. Nonell, V. Marchán.
**J. Org. Chem.** *3* (2018) 1185-1195.

80. *Generation and reactions of an octacyclic hindered pyramidalized alkene.*
T. Ginex, P. Camps, D. Lozano, C. Barbaraci, M. Font-Bardia, F. J. Luque, C. Estarellas.
**J. Org. Chem.** *83* (2018) 5420-5430.

81. *A definition of the magnetic transition temperature using valence bond theory.*
J. Jornet-Somoza, M. Deumal, J. Borge, M. A. Robb.
**J. Phys. Chem. A** *122* (2018) 2168-2177.

82. *Post-B3LYP functionals do not improve the description of magnetic coupling in Cu(II) dinuclear complexes.*
R. Costa, D. Reta, I. De P. R. Moreira, F. Illas.
**J. Phys. Chem. A** *122* (2018) 3423-3432.

83. *Matildite contact with media: first-principles study of $AgBiS_2$ surfaces and nanoparticle morphology.*
F. Viñes, G. Konstantatos, F. Illas.
**J. Phys. Chem. B** *122* (2018) 521-526.

84. *DFT-based adsorption isotherms for pure and flue gas mixtures on Mg-MOF-74. Application in $CO_2$ capture swing adsorption processes.*
G. Alonso, D. Bahamon, F. Keshavarz, X. Giménez, P. Gamallo, R. Sayós.
**J. Phys. Chem. C** *122* (2018) 3945-3957.

85. *Properties of single oxygen vacancies on a realistic $(TiO_2)_{84}$ nanoparticle: a challenge for density functionals.*
Á. Morales-García, O. Lamiel-García, R. Valero, F. Illas.
**J. Phys. Chem. C** *122* (2018) 2413-2421.

86. *Understanding W doping in wurtzite ZnO.*
F. Viñes, A. Iglesias-Juez, M. Fernández-García, F. Illas.
**J. Phys. Chem. C** *122* (2018) 19082-19089.

87. *Assessing the performance of Cobalt-phthalocyanine nanoflakes as molecular catalysts for Li-promoted oxalate formation in Li-$CO_2$-oxalate batteries.*
M. Goodarzi, F. Nazari, F. Illas.
**J. Phys. Chem. C** *122* (2018) 25776-25784.

88. *Diversity of adsorbed hydrogen on the TiC(001) surface at high coverages.*
P. J. Ramirez, S. T. Bromley, F. Illas, F. Viñes, J. A Rodríguez.
**J. Phys. Chem. C** *122* (2018) 28013-28020.

89. *Combining theory and experiment for multitechnique characterization of activated $CO_2$ on transition metal carbide (001) surfaces.*
C. Kunkel. F. Viñes, P. J. Ramírez, J. A. Rodriguez, F. Illas.
**J. Phys. Chem. C** (2018) doi: 10.1021/acs.jpcc.7b12227

90. *Surface activity of early transition metal oxycarbides: $CO_2$ adsorption case study.*
C. Kunkel. F. Viñes, F. Illas.
**J. Phys. Chem. C** (2018) doi: 10.1021/acs.jpcc.8b11942

91. *Oxygen reduction reaction: rapid prediction of mass activity of nanostructured platinum electrcatalysts.*
M. Rück, A. Bandarenka, F. Calle-Vallejo, A. Gagliardi.
**J. Phys. Chem. Lett.** *9* (2018) 4463-4468.

92. *Electronic, bonding, linear, and nonlinear optical properties of $Na_2MGe_2Q_6$ (M=Cd, Zn, Hg; Q=S, Se), $Na_2ZnSi_2S_6$, and $Na_2ZnSn_2S_6$ two metal-mixed chalcogenide compounds.*
R. Mahiaoui, T. Ouahrani, A. Chikhaoui, Á. Morales-García, A. H. Reshak.
**J. Phys. Chem. Solids** *119* (2018) 220-227.

93. *Role of lattice oxygen content and Ni geometry in the oxygen evolution activity of the Ba-Ni-O system.*
M. Retuerto, F. Calle-Vallejo, L. Pascual, P. Ferrer, Á. García, J. Torrero, D. Gianolio, J. L. G. Fierro, M. A. Peña, J. A. Alonso, S. Rojas.
**J. Power Sources** *404* (2018) 56-63.

94. *Donor-anion interactions in quarter-filled low-dimensional organic conductors.*
J. P. Pouget, P. Alemany, E. Canadell.
**Mater. Horiz.** *5* (2018) 590-640.

95. *Breakthroughs in medicinal chemistry: new targets and mechanisms, new drugs, new hopes-2.*
D. Muñoz-Torrero, A. A. Mangoni, H. Liu, C. Hulme, J. Rautio, R. Karaman, M. E. de Sousa, K. Prokai-Tatrai, J.-M. Sabatier, C. Siciliano, F. J. Luque, G. Kokotos, R. Ragno, S. Collina, C. Guillou, M. Gütschow, L. A. Agrofolio.
**Molecules** *65* (2018) 1-9.

96. *Newton trajectories for the tilted Frenkel-Kontorova model.*
W. Quapp, J. M. Bofill.
**Mol. Phys.** (2018) doi: 10.1080/00268976.2019.1576930

97. *Stability of mixed-oxide titanosilicates: dependency on size and composition from nanocluster to bulk.*
A. Cuko A, M. Calatayud, S. T. Bromley.
**Nanoscale** *10* (2018) 832-842.

98. *Properties of hydrated $TiO_2$ and $SiO_2$ nanoclusters: dependence on size, temperature and water vapour pressure.*
A. Cuko, A. M. Escatllar, M. Calatayud, S. T. Bromley.
**Nanoscale** *10* (2018) 21518-21532.

99. *Long distance electron transfer through the aqueous solution between redox partner proteins.*
A. Lagunas, A. Guerra-Castellano, A. Nin-Hill, I. Díaz-Moreno, M. A. de la Rosa, J. Samitier, C. Rovira, P. Gorostiza.
**Nat. Commun.** *9* (2018) 5157-5163.

100. *Palladium-mediated enzyme activation suggests multiphase initiation of glycogenesis.*
M. K. Bilyard, H. Bailey, L. Raich, M. Gafitescu, T. Machida, J. Iglesias-Fernández, S. S. Lee, C. D. Spicer, C. Rovira, W. W. Yue, B. G. Davis.
**Nature** *563* (2018) 235-240.

101. *The role of metal/oxide interfaces for long-range metal particle activation during CO oxidation.*
Y. Suchorski, S. M. Kozlov, I. Bespalov, M. Datler, D. Vogel, Z. Budinska, K. M. Neyman, G. Rupprechter.
**Nature Mater.** *17* (2018) 519-522.

102. *Structure, magnetic properties and DFT calculations of azido-copper(II) complexes with different azido-bonding, nuclearity and dimensionality.*
S. S. Massoud, M. M. Henary, L. Maxwell, A. Martín, E. Ruiz, R. Vicente, R. C. Fischer, F. A. Mautner.
**New J. Chem.** *42* (2018) 2627-2639.

103. *Els plastòmers.*
O. Güell, F. Mas.
**Notícies per a Químics** *479* (2018) 16-19.

104. *El carbonat de calci: molt més que un filler.*
O. Güell, F. Mas.
**Notícies per a Químics** *478* (2018) 21-26.

105. *Zn(II) byproduct enhances the Cu-catalyzed cross-coupling of bromozinc. Difluorophosphonate with Iodobenzoates: A DFT Study.*
J. Jover.
**Organometallics** *37* (2018) 327-336.

106. *Role of ring ortho substituents on the configuration of carotenoid polyene chains.*
M. Kim, H. Jung, A. C. Aragonès, I. Díez-Pérez, K.-H. Ahn, W.-J. Chung, D. Kim, S. Koo.
**Org. Lett.** *20* (2018) 493-496.

107. *Quantum-mechanical simulations of pressure effects on $MgIn_2S_4$ polymorphs.*
S. Belarouci, T. Ouahrani, N. Benabdallah, Á. Morales-García, R. Franco.
**Phase Transit.** *91* (2018) 759-771.

108. *Vibrational energy relaxation dynamics of diatomic molecules inside superfluid helium nanodroplets. The case of the $I_2$ molecule.*
A. Vilà, M. Paniagua, M. González.
**Phys. Chem. Chem. Phys.** *20* (2018) 118.

109. *Theoretical evidence for the direct $^3$MLCT-HS deactivation in the light-induced spin crossover of Fe(II)- polypyridyl complexes.*
C. Sousa, M. Llunell, A. Domingo, C. de Graaf.
**Phys. Chem. Chem. Phys.** *20* (2018) 2351-2355.

110. *On the $H_2$ interaction on transition metal adatoms supported on graphene: a systematic density functional theory.*
M. Manadé, F. Viñes, A. Gil, F. Illas.
**Phys. Chem. Chem. Phys.** *20* (2018) 3819-3823.

111. *Triarylmethyl-based 2D covalent networks: virtual screening of chemical functionalisation for optimising strain-induced property control.*
I. Alcon, S. T. Bromley.
**Phys. Chem. Chem. Phys.** *20* (2018) 5028-5035.

112. *The reactivity of the cyclopropyl cyanide in Titan's atmosphere: a possible pre-biotic mechanism*.
E. López, D. Ascenzi, P. Tosi, J. M. Bofill, J. de Andrés, M. Albertí, J. M. Lucas, A. Aguilar.
**Phys. Chem. Chem. Phys.** *20* (2018) 6198-6210.

113. *On the prediction of core level binding energies in molecules, surfaces and solids.*
F. Viñes, C. Sousa, F. Illas.
**Phys. Chem. Chem. Phys.** *20* (2018) 8403-8410.

114. *Two-dimensional nitrides as highly efficient potential candidates for $CO_2$ capture and activation.*
R. Morales-Salvador, Á. Morales-García, F. Viñes, F. Illas.
**Phys. Chem. Chem. Phys.** *20* (2018) 17117-17124.

115. *Reliable and computationally affordable prediction of the energy gap of $(TiO_2)_n$ ($10 \leq n \leq 563$) nanoparticles from density functional theory.*
Á. Morales-García, R. Valero, F. Illas.
**Phys. Chem. Chem. Phys.** *20* (2018) 18907-18911.

116. *The magnetic fingerprint of dithiazolyl-based molecule magnets.*
T. Francese, J. Ribas-Arino, J. J. Novoa, R. W. A. Havenith, R. Broer, C. de Graaf, M. Deumal.
**Phys. Chem. Chem. Phys.** *20* (2018) 20406-20416.

117. *$CO_2$ interaction with violarite ($FeNi_2S_4$) surfaces: a dispersion-corrected DFT study.*
S. Posada-Pérez, D. Santos-Carballal, U. Terranova. A. Roldan, F. Illas, N. H. De Leeuw.
**Phys. Chem. Chem. Phys.** *20* (2018) 20439-20446.

118. *Robustness of surface activity electronic-structure based descriptors of transition metals.*
L. Vega, B. Martínez, F. Viñes, F. Illas.
**Phys. Chem. Chem. Phys.** *20* (2018) 20548-20554.

119. *Determination of the protonation preferences of bilin pigments in cryptophyte antenna complexes.*
M. Corbella, Z. S. D. Toa, G. D. Scholes, F. J. Luque, C. Curutchet.
**Phys. Chem. Chem. Phys.** *20* (2018) 21404-21416.

120. *Tuning transition metal carbides activity by surface metal alloying: case study on $CO_2$ capture and activation.*
M. López, L. Broderick, J. J. Carey, F. Viñes, M. Nolan, F. Illas.
**Phys. Chem. Chem. Phys.** *20* (2018) 22179-22186.

121. *How abasic sites impact hole transfer dynamics in GC-rich DNA sequences.*
M. Corbella, A. A. Voityuk, C. Curutchet.
**Phys. Chem. Chem. Phys.** *20* (2018) 23123-23131.

122. *Tropospheric oxidation of methyl hydrotrioxide ($CH_3OOOH$) by hydroxyl radical.*
J. M. Anglada, A. Solé.
**Phys. Chem. Chem. Phys.** *20* (2018) 27406-27417.

123. *Quantum-classical dynamics of the capture of neon atoms by superfluid helium nanodroplets.*
M. Blancafort-Jorquera, A. Vilà, M. González.
**Phys. Chem. Chem. Phys.** *20* (2018) 29737.

124. *Ab initio electronic structure calculations of entire blue copper azurins.*
C. Romero-Muñiz, M. Ortega, J. G. Vilhena, I Díez-Pérez, J. C. Cuevas, R. Pérez, L. A. Zotti.
**Phys. Chem. Chem. Phys.** *20* (2018) 30392-30402.

125. *Modeling and subtleties of K-Ras and calmodulin interaction.*
E. Garrido, J. Lázaro, M. Jaumot, N. Agell, J. Rubio-Martinez.
**PLoS Comput. Biol.** *14* (2018) e1006552.

126. *Coupling of charge regulation and conformational equilibria in linear weak polyelectrolytes: treatment of long range via effective short-ranged and ph-dependent interaction parameters.*
P. M. Blanco, S. Madurga, F. Mas, J. L. Garcés.
**Polymers** *10* (2018) 811.

127. *Coupling of charge regulation and conformational equilibria in linear weak polyelectrolytes: treatment of long range via effective short-ranged and pH-dependent interaction parameters.*
P. M. Blanco, S. Madurga, F. Mas, J. L. Garcés.
**Polymers** *10* (2018) 811.

128. *SABER 2.0 a CTEM. Correcció recompensada i continguts – Estratègies pràctiques d'aprenentatge actiu.*
L. Arévalo, P. Gamallo, X. Giménez.
**REIRE** *11* (2018) 84 doi:10.1344/reire2018.11.220911

129. *Estructura electrònica i propietats de sistemes multifuncionals: materials derivats del bisditiazolil.*
C. Roncero, M. Deumal, J. Ribas, I. de P. R. Moreira.
**Revista de la Societat Catalana de Química** *17* (2018) 86-95.

130. *Structure and reducibility of doped by yttrium cerium dioxide nanoparticles and (111) surface.*
H. A. Aleksandrov, I. Z. Koleva, K. M. Neyman, T. Tabakova, G. N. Vayssilov.
**RSC Adv.** *8* (2018) 33728-33741.

131. *Solvation-guided design of fluorescent probes for discrimination of amyloids.*
K. J. Cao, K. M. Elbel, J. L. Cifelli, J. Cirera, C. J. Sigurdson, F. Paesani, E. A. Theodorakis, J. Yang.
**Sci. Rep.** *8* (2018) 6950.

132. *Electrostatic tuning of the ligand binding mechanism by Glu27 in nitrophorin 7.*
S. Abbruzzetti, A. Allegri, A. Bidon-Chanal, H. Ogata, G. Soavi, G. Cerullo, S. Bruno, C. Montali, F. J. Luque, C. Viappiani.
**Sci. Rep.** *8* (2018) 10855.

133. *Macromolecular diffusion in crowded media beyond the hard-sphere model.*
P. M. Blanco, J. L. Garcés, S. Madurga, F. Mas.
**Soft Matter** *14* (2018) 3105-3114.

134. *Exploring potential energy surfaces with gentlest ascent dynamics in combination with the shrinking dimer method and Newtonian dynamics.*
G. Albareda, J .M. Bofill, , I. de P. R. Moreira, W. Quapp, J. Rubio-Martínez.
**Theor. Chem. Acc.** *137* (2018) 73.

135. *How Au outperforms Pt in the catalytic reduction of methane towards ethane and moleculer hydrogen.*
J. I. Martínez, F. Calle-Vallejo, P. L. De Andrés.
**Top. Catal.** *61* (2018) 1290-1299.

136. *Electronic energy transfer in biomacromolecules.*
L. Cupellini, M. Corbella, B. Mennucci, C. Curutchet.
**WIREs Comput. Mol. Sci.** (2018) doi:10.1002/wcms.1392

## BOOK CHAPTERS AND PROCEEDINGS

1. *Oxygen evolution reaction catalyzed by cost-effective metal oxides.*
   O. Díaz-Morales, F. Calle-Vallejo.
   **Encyclopedia of Interfacial Chemistry** *edited by K. Wandelt* (Elsevier, The Netherlands) 2018.

2. *Modeling realistic titania nanoparticles.*
   K. C. Ko, J. Y. Lee, F. Illas.
   **Fronteirs of Nanoscience, Computational Modelling of Nanoparticles** *edited by S. T. Bromley and S. M. Woodley* (Elsevier, The Netherlands) 2018.

3. *Simulating heterogeneous catalysis on metallic nanoparticles: from under-coordinated sites to extended facets.*
   F. Viñes.
   **Fronteirs of Nanoscience, Computational Modelling of Nanoparticles** *edited by S. T. Bromley & S. M. Woodley* (Elsevier, The Netherlands) 2018.

4. *Plastics and biodegradation: what is a bioplastic?*
   O. Güell, F. Mas.
   **Hands-on Science. Advancing Science. Improving Education** (The Hand-on Science Network, Portugal) p. 306-308, 2018.

5. *Pt-$CeO_2$ catalysts for fuel cell applications: from surface science to electrochemistry.*
   Y. Lykhach, O. Brummel, A. Bruix, S. Fabris, I. Matolínová, V. Matolín, K. M. Neyman, J. Libuda.
   **Encyclopedia of Interfacial Chemistry: Surface Science and Electrochemistry, vol. 2,** p. 189-201*, edited by K. Wandelt* (Elsevier, Oxford) 2018.

6. *Electron transport through peptides and blue-Copper azurins*
   L. A. Zotti, M. P. Ruiz, A. C. Aragonés, N. Camarero, J. G. Vilhena, M. Ortega, R. Perez, J. C. Cuevas, P. Gorostiza, I. Diéz-Pérez.
   **APS Meeting Abstracts** *edited by APS* (Bulletin of the American Physical Society, USA) 2018.

7. *Chlorophylls in a protein environment: How to calculate their spectral and redox properties (from MO to DFT).*
   C. Curutchet, B. Mennucci
   **Light Harvesting in Photosynthesis** *edited by R. Croce, R. van Grondelle, H. van Amerongen and I. van Stokkum* (CRC Press - Taylor and Francis Group, USA) 2018.

8. *On the use of quantum mechanical solvation continuum models in drug design: IEF/PCM-MST hydrophobic descriptors in 3D-QSAR analysis of AMPA inhibitors.*
   T. Ginex, E. Herrero, E. Gibert, F. J. Luque.
   **Theoretical and Quantum Chemistry at the Dawn's End of 21st Century,** *edited by T. Chakraborty, R. Carbó-Dorca* (Apple Academic Press, USA) 2018.

9. *Effect of the solvent on the conformational behavior of the alanine dipeptide in explicit solvent simulations.*
J. Rubio-Martínez, J. J. Perez.
**Theoretical and Quantum Chemistry at the Dawn's End of 21st Century,** *edited by T. Chakraborty, R. Carbó-Dorca* (Apple Academic Press, USA) 2018.

10. **Computational Modelling of Nanoparticles***, Vol 12. Frontiers of Nanoscience, edited by S. T. Bromley and S. M. Woodley* (Elsevier, UK) 2018.

## III.3 OTHER ACTIVITIES

### DOCTORALS THESES 2018

1. *Electroreduction of Nitratre and Carbon Dioxide on Cooper Electrodes.*
   **Elena Pérez-Gallent**
   Leiden Institute of Chemistry, Leiden University.
   February 2018.

2. *Heterogeneous Catalysis of Green Chemistry Reactions on Molybdenum Carbide Based Catalysts.*
   **Sergio Posada Pérez**
   Supervisor/s: F. Illas and F. Viñes
   Facultat de Química, Universitat de Barcelona.
   March 2018.

3. *Rational Chemical Design of Triarylmethyl-Based Devices and 2D Materials.*
   **Isaac Alcón Rovira**
   Facultat de Química, Universitat de Barcelona.
   March 2018.

4. *Quantum Confinement of Gaseous Molecules in Nanostructures: Effects on the Dynamics and Internal Structure.*
   **Manel Mondelo Martell**
   Programa de Doctorat de Nanociències.
   Facultat de Química, Universitat de Barcelona.
   June 2018.

5. *Simulación molecular aplicada a inhibidores de 11β hidroxiesteroide deshidrogenasa tipo 1 y efecto de temperatura en Citoglobina.*
   **Constantí Seira Castan**
   Programa de doctorat en Recerca, Desenvolupament i Control de Medicaments.
   Facultat de Farmàcia i Ciències de l'Alimentació, Universitat de Barcelona.
   July 2018.

6. *Modelització multiescala del paper de l'entorn en processos de transferència de càrrega i d'energia en biomolècules.*
   **Marina Corbella Morató**
   Programa de Doctorat en Recerca, Desenvolupament i Control de Medicaments.
   Facultat de Farmàcia i Ciències de l'Alimentació, Universitat de Barcelona.
   July 2018.

7. *Unveiling protein-substrate interactions and conformations that influence catalysis in carbohydrate-active enzymes.*
**Lluís Raich Armendáriz**
Química Teòrica i Modelització Computacional
Facultat de Química, Universitat de Barcelona.
July 2018.

8. *Modelling Nano-oxide Materials with Technolgical and Environmental Relevance: Silica, Titania and Titanosilicates.*
**Andi Cuko**
Facultat de Química, Universitat de Barcelona.
September 2018.

9. *Cathodic Corrosion.*
**Thomas J. P. Hersbach**
Leiden Institute of Chemistry, Leiden University.
December 2018.

## MASTERS THESES 2018

1. *Contribution to the Study of Methyl Acetate Transesterification by Reactive Pressure-Swing Distillation.*
**Alvaro Risco Morillo**
Màster en Enginyeria Química.
Facultat de Química, Universitat de Barcelona.
February 2018.

2. *Effect of theh chemical environament on redox single-molecule contacts.*
**Mrug Upadhyay**
King's College London.
April 2018.

3. *A Molecular Dynamics investigation of Lipooligosaccharide α-galactosyltransferase C (LgtC).*
**Charlotte Madill**
Màster en Química Teòrica i Modelització Computacional.
Facultat de Química, Universitat de Barcelona.
June 2018.

4. *Surrogate model for carbon dioxide equilibrium absorption using aqueous ammonia.*
**Jesus Garcia Aspano**
Màster d'Enginyeria Ambiental.
Facultat de Química, Universitat de Barcelona.
June 2018.

5. *Surrogate Model For Carbon Dioxide Equilibrium Absorption Using Aqueous*

*Alkanolamines.*
**Laidy Diana Medina Quinquin**
Màster d'Enginyeria Ambiental.
Facultat de Química, Universitat de Barcelona.
June 2018.

6. *Chimney flue gas immission simulated using ANSYS®.*
**Yulissa Espil Sánchez**
Màster en Enginyeria Química.
Facultat de Química, Universitat de Barcelona.
June 2018.

7. *Selective allosteric inhibition of the antiapoptotic Bcl-xL and Mcl-1 proteins.*
**Cristian Privat Contreras**
Màster en Modelització Computacional Atomística i Multiescala en Física, Química i Bioquímica.
Facultat de Química. Universitat de Barcelona.
July 2018.

8. *Studies of Spin Crossover Complexes: Dispersion Effects and Troublesome Cases.*
**Francisco Alonso Gómez Mudarra**
Máster en Química de Materiales Aplicada.
Facultat de Química, Universitat de Barcelona.
July 2018.

9. *Molecular Determinats in the Interaction between Bak and BH3-only peptides: Towards the Design of Bak Activators.*
**Guillem Vila Julià**
Màster en Bioinformatics for Genomic and Drug Design.
Universitat Autònoma de Barcelona.
July 2018.

10. *Computational study of tacticity effect on polypropylene structural properties using Rotational Isomeric State model.*
**Jordi Sans Duñó**
Facultat de Química, Universitat de Barcelona.
July 2018.

11. *Theoretical Modeling of the Spin-crossover Behavior in the [Fe(1H-tetrazole)6] Metal-organic Framework.*
**Mitali Vijaykum Patel**
Màster en Química de Materials Aplicada.
Facultat de Química, Universitat de Barcelona.
July 2018.

12. *Interplay of Carbon on Transition Metal Surfaces and Nanoparticles.*
**Oriol Piqué Caufapé**
Director/s: F. Viñes
Màster en Modelització Computacional Atomística i Multiescala en Física, Química i Bioquímica.
Facultat de Química, Universitat de Barcelona.
July 2018.

13. *Computational study of the phase transition in the heterocyclic bis(1,2,3,5-dithiadiazolyl)-4,4'-biphenylene diradical.*
**Raúl Santiago Piera**
Màster en Modelització Computacional Atomística i Multiescala en Física, Química i Bioquímica.
Facultat de Química, Universitat de Barcelona.
July 2018.

14. Magnetic transition in Proton Coupled to Electron Transfer PCET anthranol/anthroxyl crystal
**Sergio Pablo García Carrillo**
Màster en Modelització Computacional Atomística i Multiescala en Física, Química i Bioquímica.
Facultat de Química, Universitat de Barcelona.
July 2018.

## SCIENTIFIC CONFERENCES AND MEETINGS 2018

**Seminaris del Departament de Química de la Universitat d'Estrasburg**
Estrasburg (France), 19 January 2018

*The complex mechanochemistry of disulfide bond reduction in alkaline solution (oral communication)*
J. Ribas

**Verdaguer Symposium**
Paris (France), 19 January 2018

*Chemical Laboratories in Art and Print (invited talk)*
S. Alvarez

**International Workshop on Oxide Surfaces (IWOX-XI)**
Granada (Spain), 22-26 January 2018

*Properties of Realistic Oxide Nanoparticles from Relativistic All Electron Density Functional Theory Based Calculations (invited talk)*
F. Illas

**18º Congreso de la Sociedad Española de Química Terapéutica: 'New perspectives in Drug Discovery'**
Salamanca (Spain), 23-26 January 2018

*Molecular dynamics simulations of AMPK mechanism of allosteric regulation by direct activators (oral communication)*
C. Estarellas, E. Fara, S. Quesada-Sánchez, A. Castro, F. J. Luque

*Molecular Natural (poly)phenols and Alzheimer's disease: Theoretical elucidation of the structural determinants for covalent amyloid beta (Aβ) inhibition (oral communication)*
T. Ginex, F. J. Luque

**Desena Trobada de Joves Investigadors dels Països Catalans**
Barcelona (Spain), 29 January 2018

*Difusió en medis d'alta ocupació macromolecular: model més enllà de l'aproximació d'esferes dures (oral communication)*
P. M. Blanco, J. L. Garcés, S. Madurga, F. Mas

**16th Iberian Meeting/ 4th ChemBio Group Meeting of the Real Sociedad de Química Española**
Barcelona (Spain), 5 February 2018

*Catalysis by natural and engineered glycosidases (invited talk)*
C. Rovira

**IV Reunión de Jóvenes Investigadores en Coloides e Interfases (JICI-IV)**
Córdoba (Spain), 8 February 2018

*Modelling polymer streching: A Statistical Mechanics approach (oral communication)*
P. M. Blanco, J. L. Garcés, S. Madurga, F. Mas

**XX Programa de Promoción de la Cultura Científica y Tecnológica**
Talavera de la Reina (Spain), 8 February 2018

*Química en la literatura: cosmogonías y química silábica (invited talk)*
S. Alvarez

**2018 Workshop on Theoretical Chemistry – Modelling of Environment Effects in Quantum Chemistry**
Mariapfarr (Austria), 20-23 February 2018

*QM/MM with polarizable embeddings (from ground state to photoinduced processes) (invited talk)*
C. Curutchet

**International Workshop on Molecular Architectonics 2018**
Osaka (Japan), 2-3 March 2018

*Charge Transport in Single-molecule wires (invited talk)*
I. Diez-Perez

**XX Programa de Promoción de la Cultura Científica y Tecnológica**
Segòvia (Spain), 12 March 2018

*Química en la literatura: cosmogonías y química silábica (invited talk)*
S. Alvarez

**32nd Molecular Modelling Workshop 2018**
Erlangen (Deutschland), 12-14 March 2018

*Hydrophobic Similarity: Application to Three-Dimensional Molecular Overlays with PharmScreen (oral communication)*
J. Vazquez, A. Deplano, A. Herrero, T. Ginex, E. Gibert, O. Rabal, J. Oyarzabal, E. Herrero, F. J. Luque

**255th American Chemical Society**
New Orleans (USA), 18-22 March 2018

*Hydrophobic similarity between molecules: Application to three-dimensional molecular overlays with PharmScreen (oral communication)*
J. Vazquez, A. Deplano, A. Herrero, E. Gibert, T. Ginex, O. Rabal, J. Oyarzabal, E. Herrero, F. J. Luque

*Computational modelling of the ligand tuning effect over the Transition Temperature in Spin-Crossover systems using Density Functional Methods (oral communication)*
J. Cirera

*Benchmarking Density Functional Methods for Calculation of State Energies of First Row Spin-Crossover Molecules (oral communication)*
J. Cirera

*Alkyl groups as electron density donors in $\pi$-hole bonding (oral communication)*
J. Echeverría

*Frustrated Lewis Trios and long-range hole interactions (oral communication)*
J. Echeverría

**Polymers 2018: Design, Function and Application**
Barcelona (Spain), 21 March 2018

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

**H2020 Materials Networking School**
Sofia (Bulgaria), 21 March 2018

*Computer-aided analysis of the structure and stability of B-DNA: towards the design of supramolecular self-assembling materials (invited talk)*
J. Poater

*Studying charge transport in Biomolecular Interfaces (invited talk)*
I. Diez-Perez

**Predictive Catalysis: Transition-Metal Reactivity by Design (Girona Seminar 2018)**
Girona (Spain), 3 April 2018

*Structure and stability of B-DNA model systems in non-terran bio-solvents (poster)*
J. Poater, T. A. Hamlin, C. F. Guerra, F. M. Bickelhaupt

**X Jornadas de Jóvenes Investigadores en Física Atómica y Molecular (J²IFAM)**
Barcelona (Spain), 3-6 April 2018

*Compactness and d-band Filling Effect on Chemical Descriptors for Transition Metals (oral communication)*
B. Martínez Díaz, L. Vega, F. Viñes

*Post-Combustion $CO_2$ gas Separation with Zeolites (oral communication)*
H. Prats García

*Tuning Acitivity of Transition Metal Carbides by Surface Metal Alloying: Case of Study of $CO_2$ Capture (oral communication)*
M. López, F. Viñes, F. Illas

*Activation of the $CO_2$ Molecule on MXenes Nitrides (oral communication)*
R. Morales-Salvador, Á. Morales-García, F. Viñes

**X Conference of Young Scientists in Atomic and Molecular Physics**
Barcelona (Spain), 4 April 2018

*Diffusion in crowded media: Modelling beyond the hard-sphere approximation (oral communication)*
P. M. Blanco, J. L. Garcés, S. Madurga, F. Mas

**22nd Topical Meeting of the International Society of Electrochemistry**
Tokyo (Japan), 15-18 April 2018

*Optimizing Platinum Electrocatalysts for Various Reactions by Means of Coordination-Activity Plots (oral communication)*
F. Calle-Vallejo

**Quantum Frontiers and Fundamentals: Experimental Studies and Theoretical Ramifications**
Bangaluru (India), 30 April – 4 May 2018

*Non-universality of quantum dynamics computed from time-correlation functions (invited talk)*
X. Oriols, G. Albareda, D. Pandey

**Lectures in UAB**
Barcelona (Spain), 3 May 2018

*How Far Quantum Chemical Models Can Go On Predicting Properties of Realistic Semiconducting Oxide Nanoparticles? (invited seminar)*
F. Illas

**Masterquímica XIV**
Barcelona (Spain), 9 May 2018

*Precisió dels Funcionals de la Densitat en la Descripció de les Propietats Superficials del Metalls de Transicin (poster)*
L. Vega, J. Ruvireta, F. Viñes, F. Illas

*Estudi computacional de l'efecte de la tacticitat en les propietats conformacionals del polipropilè (poster)*
J. Sans, P. M. Blanco, S. Madurga, J. L. Garcés, F. Mas.

**Seminarios de la Universidad de Antioquia**
Medellín (Colombia), 9 May 2018

*Transition Metal Carbides against Global Warming (invited talk)*
F. Viñes

**XX Programa de Promoción de la Cultura Científica y Tecnológica**
Madrid (Spain), 10 May 2018

*Química en la literatura: cosmogonías y química silábica (invited talk)*
S. Alvarez

**5th International School-Conference on Catalysis for Young Scientists "Catalyst Design: From Molecular to Industrial Level"**
Moscow (Rusia), 20-23 May 2018

K. M. Neyman *(scientific committee)*

**11th European School on Molecular Nanoscience (EsMolNa)**
Tenerife (Spain), 20-25 May 2018

*Tunneling Transport in Curcuminoid Systems (invited talk)*
E. Ruiz

**HPC for next generation nanomaterials & nanodevices engineering**
Bellaterra (Spain), 30-31 May 2018

*Computer simulation of biological processes: enzyme catalysis (keynote talk)*
C. Rovira

*High Performance Computing for the Understanding of Realistic $TiO_2$ and ZnO Nanoparticles (poster)*
Á. Morales-García, O. Lamiel-García, A. Macià-Escatllar, K. C. Ko, R. Valero, F. Viñes, S. T. Bromley, F. Illas

**IX IQTCUB Symposium**
Barcelona (Spain), 1 June 2018

M. Deumal, J. Cirera *(Organization and chairpersons)*

*Understanding the origin of magnetic anisotropy in S=1/2 mononuclear transition metal complexes (invited talk)*
M. Amoza

*Electronic structure and properties of multifunctional systems: bisdithiazolyl-based materials (poster)*
C. Roncero, M. Deumal, I. P. R. Moreira, J. Ribas-Arino

*Computational Design of New Materials for Water Electrlyzers (invited talk)*
F. Calle-Vallejo

*On the Accuracy of Density Functionals in Describing Transition Metal Surface Properties (poster)*
L. Vega, J. Ruvireta, F. Viñes, F. Illas

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

*Two-Dimensional Nitrides as Highly Efficient Potential Candidates for $CO_2$ Capture and Activation (poster)*
R. Morales-Salvador, Á. Morales-García, F. Viñes, F. Illas

*To what extent do chemical descriptors behave as such? (poster)*
B. Martínez, L. Vega, F. Viñes

*$H_2$ dissociation on transition metal carbide surfaces (poster)*
J. J. Piñero, P. J. Ramírez, S. T. Bromley, F. Illas, F. Viñes, J. A. Rodriguez

*A theoretical approach to the reaction dynamics involving superfluid helium nanodroplets. The production of $Ne_2@(^4He)_{N'}$ from $Ne + Ne@(^4He)_N$ (poster)*
M. Blancafort, A. Vilà, M. González

*Vibrational energy relaxation of diatomics in superfluid helium nanodroplets. Quantum dynamics approach and application to the $I_2$ molecule (poster)*
A. Vilà, M. Paniagua, M. González

*Dynamics of the $O + D_2^+ \rightarrow OD^+ + D$ gas phase reaction. QCT study on the ground PES and comparison with the experiment (poster)*
P. Gamallo, M. Paniagua, M. González

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

*Estudi computacional de l'efecte de la tacticitat en les propietats conformacionals del polipropilè (poster)*
J. Sans, P. M. Blanco, S. Madurga, J. L. Garcés, F. Mas

*Finding the optimum cation content in faujasites for post-combustion $CO_2$ capture, and application in swing adsorption processes (pòster)*
D. Bahamon, H. Prats G. Alonso, X. Giménez, P. Gamallo, R. Sayós

**Non-Adiabatic Quantum Dynamics: From Theory to Experiments**
Lausanne (Switzerland), 2-7 June 2018

*Ab-initio nonadiabatic dynamics without Born-Oppenheimer potential-energy surfaces (invited talk)*
G. Albareda

**NoSIC 8 (Not Strictly Inorganic Chemistry)**
Prullans (Spain), 6-8 June 2018

S. Álvarez *(chairman)*

*Photographers of Chemistry (invited talk)*
S. Alvarez

**Theoretical Studies of Magnetic Systems: Methodological Developments and Applications, Satellite Meeting of 16th International Conference Quantum Chemistry (ICQC)**
Toulouse (France), 13-16 June 2018

*Room Temperature Magnetoresistance in Single-Molecule Metalloporphyrin-Based Devices (invited talk)*
E. Ruiz

**2nd International Symposium on Single-Atom Catalysis (ISSAC2)**
Beijing (China), 15-18 June 2018

K. M. Neyman *(chairman)*

*Progress in density-functional modelling of ceria-based nanomaterials for single-atom catalysis (keynote talk)*
K. M. Neyman

**Theormag2018 (International Conference Quantum Chemistry ICQC Satellite)**
Toulouse (France), 18-23 June 2018

*On the importance of models for modeling magnetism (oral communication)*
M. Deumal

**President's Meeting of the International Society of Quantum Biology and Pharmacology**
Barcelona (Spain), 19-21 June 2018

*Assessing drug-binding through simulations of electronic energy transfer (oral communication)*
C. Curutchet

**Photoinduced Processes in Embedded Systems**
Pisa (Italy), 24-27 June 2018

*Assessing drug-binding through simulations of electronic energy transfer (oral communication)*
C. Curutchet

**International Congress of Theoretical Aspects in Catalysis – ICTAC 2018**
Los Ángeles (USA), 24-28 June 2018

*$CO_2$ Capture & Conversion Using Transition Metal Carbide Systems (oral communication)*
F. Viñes, C. Kunkel. Á. Morales-Garcia, F. Illas

**Cancer and Metabolism 2018**
Cambridge (UK), 25 June 2018

*Metabolic characterization of castration-resistant prostate cancer (CRPC): Metabolic phenotype associated with metastatic progression*
C. Balcells, I. Marín de Mas, M. Tarrado-Castellarnau, S. Marín, P. de Atauri, J. Centellas, F. Mas, T. M. Thompson, M. Cascante

**3rd International Conference "Fundamentals and applications of cerium dioxide in catalysis"**
Barcelona (Spain), 25-27 June 2018

K. M. Neyman *(scientific committee)*

*Density functional studies of ceria-based nanostructures for catalysis: Recent progress and challenges (oral communication)*
K. M. Neyman

**IUVSTA-ASEVA workshop "Physics and Chemistry of Nanoscale Oxide Systems"**
Ávila (Spain), 1-6 July 2018

*Density functional studies of ceria-based nanostructures: Recent progress and challenges (invited talk)*
K. M. Neyman

*Tracking The Properties Of Oxides From Nanoscale To Bulk: Implications For Nano-Oxide Based Technologies (invited talk)*
S. T. Bromley

**Invited seminar at The Hebrew University of Jerusalem**
Jerusalem (Israel), 2 July 2018

*Bio-inspired Single-molecule Junctions*
I. Diez-Perez

**Invited seminar at The Weissman Institute of Science**
Rehovot (Israel), 5 July 2018

*Bio-inspired Single-molecule Junctions*
I. Diez-Perez

**European Colloquium on Inorganic Reaction Mechanisms (ECIRM)**
Barcelona (Spain), 8-11 July 2018

*Zn(II) byproduct promotion of the Cu-catalyzed cross-coupling of bromozinc-difluorophosphonate with iodobenzoates (oral communication)*
J. Jover

*Phosphatase Activity of Binuclear Copper(II) Complexes: The Role of the Counteranions (poster)*
G. Aullón

**Advanced Materials Workshop**
Duni (Bulgaria), 11-14 July 2018

*Atomic arrangement of PtCu bimetallic nanoparticles determined using topological energy expressions (oral communication)*
L. Vega, K. M. Neyman, F. Viñes

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

**XXXIV Annual Meeting of the Reference Network in Theoretical and Computational Chemistry (XRQTC)**
Barcelona (Spain), 12 July 2018

G. Aullón, J.M. Bofill, J. Poater, C. Sousa *(organization and chairpersons)*

*$H_2$ dissociation on transition metal carbide surfaces (poster)*
J. J. Piñero, P. J. Ramírez, S. T. Bromley, F. Illas, F. Viñes, J. A. Rodriguez

*Quantum-classical approach to the reaction dynamics in superfluid helium nanodroplets. The Ne + Ne@($^4He$)$_N$ → $Ne_2$@($^4He$)$_{N'}$ + (N-N')$^4He$ reaction (oral communication)*
M. Blancafort, A. Vilà, M. González

*A computational study of tacticity effect using RIS model (oral communication)*
J. Sans, P. M. Blanco, S. Madurga, J. L. Garcés, F. Mas

**Frontiers and challenges of computing metals for biochemical, medical and technological Applications. CECAM workshop**
Paris (France), 11 July 2018

*The reaction mechanism of catalase-peroxidases (invited talk)*
C. Rovira

**Hands of Science (HSCI2018)**
Barcelona (Spain), 12 July 2018

*Plastics and biodegradation: what is a bioplastic? (oral communication)*
O. Güell, F. Mas

**29th International Carbohydrate Symposium**
Lisbon (Portugal), 15 July 2018

*Unusual catalytic itineraries of glycosidases unveiled from QM/MM metadynamics simulations (oral communication)*
C. Rovira

**28th International Conference in Organometallic Chemistry (ICOMC)**
Florence (Italy), 15-20 July 2018

*Electronic and steric control of the Spin-Crossover behavior in [$(Cp^R)_2Mn$] manganocenes (invited talk)*
J. Cirera

**11th Congress on Electronic Structure: Principles and Aplications (ESPA)**
Toledo (Spain), 17-19 July 2018

*Magnetoresistance in Single-Molecule Devices (invited talk)*
E. Ruiz

*Magnetic Fingerprint of Dithiazolyl-Based Molecule Magnets (oral communication)*
M. Deumal

*Location of optimal bond breaking points on potential energy surfaces (poster)*
J. M. Bofill, J. Ribas-Ariño, S. P. García, W. Quapp

*Gentlest Ascent Dynamics combined with Shrinking Dimer Method and Newtonian Dynamics and efficient way to explore Potential Energy Surfaces (poster)*
J. M. Bofill, J. Ribas-Ariño, R. Valero, G. Albareda, I. de P.R. Moreira, W. Quapp

*DFT-based adsorption isotherms for pure and flue gases including $SO_2$ poisoning on Mg-MOF-74 (comunicació oral)*
G. Alonso, D. Bahamón, F. Keshavarz, X. Giménez, P. Gamallo, R. Sayós

*$CO_2$ capture via swing adsorption processes using faujasites (pòster)*
H. Prats, D. Bahamón, G. Alonso, P. Gamallo, X. Giménez, R. Sayós

*Understanding the gas solubility behaviour in ionic liquids combining different molecular modelling tools: soft-SAFT and COSMO-RS (pòster)*
G. Alonso, P. Gamallo, R. Sayós, F. Llovell

**25th years of macromolecular crystallography in Barcelona**
Barcelona (Spain), 18 June 2018

*The Fita-Rossmann catalytic mechanism (invited talk)*
C. Rovira

**ISQBP President's meeting 2018**
Barcelona (Spain), 19 June 2018

*Catalysis by natural and engineered glycosidases (invited talk)*
C. Rovira

**18th IEEE International Conference on Nanotechnhology - IEEE Nano 2018**
Cork (Ireland), 23-26 July 2018

*$CO_2$ Capture & Conversion Using Transition Metal Carbide Systems (oral communication)*
F. Viñes, C. Kunkel. Á. Morales-Garcia, F. Illas

*Tracking the Properties of Oxide Materials from Nanoscale to Bulk (conferència convidada)*
S. T. Bromley

**II Jornadas españolas de biocatálisis 2018**
Oviedo (Spain), 25 July 2018

*How carbohydrate-active enzymes work. Insight from computer simulation (invited talk)*
C. Rovira

**CECAM, Biomolecular Electronics**
Madrid (Spain), 27 July-31 August 2018

*Engineering Single-Protein Junctions (invited talk)*
I. Diez-Perez

**MESM2018 International Conference on Molecular Electronic Structure**
Metz (France), 28 July-31 August 2018

J. M. Bofill *(organization and chairman)*

*Biradical Species induced by Valence Tautomerism: a challenge for Electronic Structure Methods (oral communication)*
I. de P. R. Moreira, J . M. Bofill, R. Valero, G. Albareda

**43rd International Conference on Coordination Chemistry (ICCC2018)**
Sendai (Japan), 30 July – 4 August 2018

*Magnetoresistance at Room Temperature in Single-Molecule Metalloporphyrin-Based Devices (invited talk)*
E. Ruiz

*The mechanism of the magnetic bistability in CuII(hfac)2LBu (conferència convidada)*
J. J. Novoa

**Italian Physical Chemistry Society**
Bologna (Italy), 4 August 2018

*Studying Charge transport in Biological Molecular Moieties (keynote talk)*
I. Diez-Perez

**Symposium "Nano-alloys: Theory, Synthesis & Characterization", XXVII International Materials Research Congress**
Cancun (Mexico), 20-21 August 2018

K. M. Neyman *(organization)*

**21st Conference on Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction**
Prague (Czech Republic), 26-27 August 2018

Sessió "Process Modelling"
J. Bonet *(scientific committee and chairman)*

*Surrogate model for carbon dioxide equilibrium absorption using aqueous monoethanolamine (oral communication)*
V. Plesu, J. Bonet, A.-E. Bonet-Ruiz, A. Chavarria, P. Iancu, J. Llorens

*Immission assessment inside an industrial ventilated room using CFD (poster)*
V. Plesu, A.-E. Bonet-Ruiz, J. Bonet, P. Iancu, J. Llorens, L.-I. Becerra

*A heuristic for extractive agent flow rate in extractive distillation (poster)*
V. Plesu, S. Cantero, A.-E. Bonet-Ruiz, J. Bonet, P. Iancu, J. Llorens

**7th EuCheMS Chemistry Congress - Molecular frontiers & global challenges**
Liverpool (UK), 26-30 August 2018

*Charge transport in bisdithiazolyl-based compounds (oral communication)*
C. Roncero

*Computational study of aluminum content tuning on FAU-type zeolites for optimal post-combustion $CO_2$ capture by swing adsorption processes (pòster)*
D. Bahamón, H. Prats, P. Gamallo, G.Alonso, X. Giménez, R. Sayós

**European Conference on Surface Science, ECOSS 34**
Aarhus (Denmark), 26-31 August 2018

*Structure and Reactivity of Interstellar Nanodust (invited talk)*
S. T. Bromley

**International Symposium on Polyelectrolytes (ISP2018)**
Wegeningen (Netherlands), 27 August 2018

*Charge regulation influence on conformational, binding and streching properties of polyelectrolytes (poster)*
P. M. Blanco, J. L. Garcés, S. Madurga, F. Mas

**XXXth General Assembly of the International Astronomical Union – Session FM10: Nano Dust in Space and Astrophysics**
Vienna (Austria), 28-29 August 2018

*Formation, Processing and Properties of Nano-silicate Dust: a Bottom-up Computatiuonal Modelling Approach (invited talk)*
S. T. Bromley

**16th International Conference on Molecule-based Magnets (ICMM)**
Rio de Janeiro (Brasil), 1-5 September 2018

*Improving Slow Spin Relaxation Properties by Encapsulation (invited talk)*
E. Ruiz

**69th Annual Meeting of the International Society of Electrochemistry**
Bologna (Italy), 2-7 September 2018

I. Díez-Pérez *(organization)*

*Importance of Solvation in Computational Electrocatalysis Models (oral communication)*
F. Calle-Vallejo

*Single-Protein Junctions (invited talk)*
I. Diez-Perez

**Second European Symposium on Chemical Bonding**
Oviedo (Spain), 3 September 2018

*Aromaticity of closo boron hydride clusters linked to polycyclic aromatic hydrocarbons via Hückel's rule (invited talk)*
J. Poater

**XXth International Conference on Oxygen Binding and Sensing Proteins (O2BIP2018)**
Barcelona (Spain), 3-6 September 2018

Elnaz Aledavood, Axel Bidon-Chanal, Leonardo Boechi, Mauro Bringas, Lula Capece, Carolina Estarellas, Darío A. Estrín, F. Javier Luque, Constantí Seira, Silvia Chellini *(organization)*

**XXXVI GEQO Congress Organometallic Chemistry Group**
Saragossa (Spain), 5-7 September 2018

*The n-π* interaction in transition metal complexes (oral communication)*
J. Echeverría

**International Conference on Stereodynamics (Stereodynamics 2018)**
Arosa (Switzerland), 5-7 September 2018

*Non-adiabatic charge transfer reactions in $N_2O(^1\Sigma^+)$ + $Na^+(^1S_o)$ collisions in the 0,50-5,00 keV laboratory energy range: An experimental study and a theoretical structure and dynamics approach (invited talk)*
J. de Andrés, J. M. Lucas, J. M. Bofill, M. Albertí, A. Aguilar

**Graphene Week 2018**
Donosti (Spain), 10-14 September 2018

*Post-graphene organic Dirac materials with tunable spin-polarised and semiconducting states (oral communication)*
S. T. Bromley

**"Advanced Materials" Workshop**
Duni (Bulgaria), 11-14 September 2018

*Understanding the origin of magnetic anisotropy in S=1/2 mononuclear transition metal complexes (oral communication)*
M. Amoza

*Density-functional modelling of nanocomposite materials for catalysis and new energy technologies (plenary conference)*
K. M. Neyman

*Oxazoline or oxazolinium ion? The protonation state and conformation of the reaction intermediate of chitinase enzymes revisited (invited talk)*
J. Coines

**VII SEEDMOL, Simpósio de Estructura Electrônica e Dinâmica Molecular**
Brasilia (Brasil), 17-21 September 2018

*Bringing Quantum Chemical Models to the Limit: Ground State and Excited State Properties of Realistic Oxide Nanoparticles (invited talk)*
F. Illas

**3rd Workshop on Magnetically Induced Currents in Molecules**
Kragujevac (Serbia), 23 September 2018

*Closo boron hydride clusters versus polycyclic aromatic hydrocarbons (invited talk)*
J. Poater

**BIO-COMP-CHEM Training School**
Bansko (Bulgaria), 24-28 September 2018

*Metalloenzymes as teaching tools for coordination chemistry: From bonding to spectroscopy (invited talk)*
J. Cirera

*A theoretical approach to the study of weak interactions in chemistry and biology (invited talk)*
J. Echeverría

**16th V.A. Fock Meeting on Quantum and Computational Chemistry**
Sochi (Rusia), 1 October 2018

*Stopping power beyond the adiabatic approximation: application to polymeric materials (invited talk)*
P. Alemany

**Ciencia en Acción**
Viladecans (Spain), 7 October 2018

*La tabla periódica, un icono cultural (invited talk)*
S. Alvarez

**ACS on Campus**
Barcelona (Spain), 18 October 2018

*Scientific Publishing in Chemistry Now and Then (invited talk)*
F. Illas, F. Viñes, L. Vega

**2nd Carbohydrate and fluorine symposium**
Poitiers (France), 18 October 2018

*An atomistic view to glycan hydrolysis by quantum mechanics/molecular dynamics (invited talk)*
C. Rovira

*Does the superacid media mimic the enzyme environment in a glycosidic reaction? computational study of the 2-deoxy-β-glucose glycosyl cation in liquid HF/$SbF_5$ (oral communication)*
A. Nin-Hill

**2nd European Conference Molecular Spintronics (ECMol), Reunió COST Molspin**
Peñíscola (Spain), 21-24 October 2018

*Magnetic effects in single-molecule junctions (invited talk)*
I. Diez-Perez

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

**XI Iberoamerican Conf. on Phase Equilibria & Fluid Props. for Process Design (EQUIFASE)**
Cordoba (Argentina), 22- 25 October 2018

*Molecular simulation study of the oil / water interface in the presence of different salts and surfactants (poster with honorific mention)*
G. Alonso, P. Gamallo, A. Mejía, R. Sayós

**HPC-Europa3 Transnational Access Meeting**
Edimburg (UK), 23 October 2018

*Noncovalent interactions involving nitrosyl ligands (invited talk)*
J. Echeverría

**Symposium in Honour of Professor Ernesto Carmona**
Sevilla (Spain), 24-25 October 2018

*Coordination Spheres within Proteins: a Shape Analysis (invited talk)*
S. Alvarez

**20th Conference of Nanoscience and Nanotecgnology**
Sofia (Bulgaria), 8 November 2018

*How to distinguish the allergens of nonallergens proteins? (oral communication)*
M. Nedyalkova, S. Madurga, F. Mas, V. Simeonov

**"Química, una Ciencia Central", Ciclo de Divulgación Científica del ISQCH (UZ-CSIC)**
Zaragoza (Spain), 14 November 2018

*Literatura de la química y química de la literatura (invited talk)*
S. Alvarez

**I Tesimarató de Química**
Barcelona (Spain), 21 November 2018

*Carburs de metalls de transició nanoestructurats com a possible catalitzadors per a l'activació del metà (oral communication)*
M. Figueras, F. Illas, F. Viñes

*Precisió dels Funcionals de la densitat en propietats superficials dels metalls de transició (oral communication)*
L. Vega, K. M. Neyman, F. Viñes

*Control de l'activitat de carburs de metalls de transició mitjançant l'aliatge metàl·lic: Captura de $CO_2$ (oral communication)*
M. López, F. Illas, F. Viñes

*Interacció del Carboni amb els Metalls de Transició (oral communication)*
O. Piqué, F. Viñes

**Aromaticity 2018**
Mayan Riviera (Mexico), 28 November 2018

*Role of aromaticity and H···H interactions in the stability of polycyclic aromatic hydrocarbons (invited talk)*
J. Poater

**Trends in enzyme catalysis. Merging theory and experiment**
Benicàssim (Spain), 29 November 2018

*An atomistic view to glycan hydrolysis by quantum mechanics/molecular dynamics (invited talk)*
C. Rovira

**Molim COST action working group 3 workshop. Ab-Initio Modelling of Molecular Processes Under Confinement**
Madrid (Spain), 3-5 December 2018

*Reactive and energy transfer processes involving atoms/molecules and superfluid helium nanodroplets (oral communication)*
M. Blancafort, A. Vilà, M. González

**CECAM Workshop "Modeling metal-based nanoparticles: environment and dynamical effects"**
Grenoble (France), 3-5 December 2018

K. M. Neyman *(chairperson)*

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

**Scanning Tiny Biology**
Barcelona (Spain), 12 December 2018

*Electrostatic Catalysis in molecular nanoscale gaps (keynote talk)*
I. Diez-Perez

## RESEARCH STAYS IN RECOGNIZED CENTERS

Albareda, G. **Max Planck Institute for the Structure and Dynamics of Matter, Hamburg (Alemanya)**
Invited visiting researcher UB invited by Prof. Angel Rubio.
January-December 2018

Albertí, M. **Univeristà di Perugia, Perugia (Itàlia)**
Research stay. Dipartimento di Chimica, Biologia e Biotecnologie.
February-July 2018

Alemany, P. **Cavendish Laboratory, University of Cambridge, Cambridge (UK)**
Invited visiting researcher UB by E. Artacho
February-October 2018

Bernuz, E. **Donostia International Physics Center, Donostia (Espanya)**
PhD research stay with Abel Carreras.
September 2018

Coines, J. **Universitat de Cagliari, Cagliari (Itàlia)**
PhD research stay with Matteo Ceccarelli.
May-July 2018

Curutchet, C. **Università di Pisa, Pisa (Itàlia)**
Invited visiting researcher UB by Benedetta Mennucci.
January 2018

Curutchet, C. **Gaussian Inc., Wallingford (CT, Estats Units)**
Invited visiting researcher UB by Giovanni Scalmani.
September-October 2018

Díez-Pérez, I. **Department of Chemistry, Kings College London**, **London (United Kingdom)**
Invited visiting researcher UB by Prof. Paula Booth.
January-December 2018

Echeverría, J. **Vrije Universiteit, Amsterdam (Països Baixos)**
HPC-Europa3 Postdoctoral stay with Prof. Célia Fonseca.
April-May 2018

Martín-Rodríguez, A. **Department of Chemistry, Kings College London**, **London (Regne Unit)**
PhD research stay with Prof. Ismael Diez-Perez.
October 2018-January 2019

| | |
|---|---|
| Neyman, K. M. | **Boreskov Institute of Catalysis Russian Academy of Sciences, Novosibirsk (Rùssia)**<br>Invited visiting researcher.<br>January-June 2018 |
| Novoa, J. J. | **Utah University, Salt Lake City (EUA)**<br>Invited visiting researcher UB by Prof. Joel S. Miller.<br>February 2018 |
| Roncero, C. | **Universität Wien, Viena (Àustria)**<br>PhD research stay with Prof. Leticia González.<br>June-July 2018 |
| Viñes, F. | **Universidad de Antioquia, Medellín (Colòmbia)**<br>Invited visiting researcher UB by A. Moreno i E. Florez.<br>October 2018 |

## PARTICIPATION IN COMPETITIVE FUNDED RESEARCH PROJECTS

*Force Fields in Redox Enzymatic Catalysis.*
I. Diez-Perez, Universitat de Barcelona
**Fields4CAT - 772391**, 2018-2023
ERC Consolidator

*Quantum Spectroscopy: exploring new states of matter out of equilibrium (Qspec-NewMat).*
A. Rubio, Max Planck Institute for the Structure and Dynamics of Matter
**ERC-2015-AdG_694097**, 2016-2021
ERC Advanced Grant

*María de Maeztu Units of Excellence 2017 for the Institut de Quimica Teòrica i Computacional.*
F. Illas, Universitat de Barcelona
**MDM 2017-0767**, 2018-2022
Ministerio de Ciencia y Universidades

*Xarxa de Referència d'R+D+I en Química Teòrica i Computacional (XRQTC).*
F. Illas, Universitat de Barcelona
2014
Departament d'Innovació, Universitats i Empresa. Generalitat de Catalunya

*Grup d'Estructura Electrònica.*
S. Alvarez, Universitat de Barcelona
**2017 SGR 1289**, 2017-2019
Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR)

*Modelització i Disseny de Sistemes Químics Radicalaris.*
J. M. Bofill, Universitat de Barcelona
**2017 SGR 348**, 2018-2020
Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR)

*Computational Materials Science Laboratory.*
F. Illas, Universitat de Barcelona
**2017 SGR 13**, 2018-2021
Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR)

*Biologia Computacional i Disseny de Fàrmacs.*
F. J. Luque, Universitat de Barcelona
**2017 SGR 1746**, 2017-2020
Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR)

*Grup de recerca consolidat: Estructura i funció en macromolècules.*
C. Rovira, Universitat de Barcelona
**2017 SGR 1189**, 2017-2020
Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR)

*ICREA Acadèmia*.
F. Illas, Universitat de Barcelona
2016-2020
Institut Català de Recerca Avançada (ICREA, Generalitat de Catalunya)

*ICREA Acadèmia*.
E. Ruiz, Universitat de Barcelona
2014-2018
Institut Català de Recerca Avançada (ICREA, Generalitat de Catalunya)

*Beca Postdoctoral Juan de la Cierva.*
J. Echeverría, Universitat de Barcelona
2016-2018
Ministerio de Economía y Competitividad (MINECO)

*Quantum Technology Emerging Community in Catalonia: QuantumCAT.*
X. Oriols, Universitat Autònoma de Barcelona
**C-IU16-001544-0002**, 2018-2020
Quantum Flagship

*Atomic ordering in bimetallic nanoparticles of fcc-type: Pt-Cu.*
K. Neyman, Universitat de Barcelona
**QCM-2018-2-0012, QCM-2018-1-0029** 2018
Red Española de Supercomputación (RES)

*Reactivity of lattice oxygen in nanostructured $CeO_2$ doped by Pt and Pd.*
K. Neyman, Universitat de Barcelona
**QCM-2018-3-0018,** 2018-2019
Red Española de Supercomputación (RES)

*Diseño computacional de pares de bases de ADN artificiales que pueden ser replicados.*
J. Poater, Universitat de Barcelona
**CTQ2016-77558-R**, 2016-2019
Ministerio de Economía y Competitividad (MINECO)

*Estudio Computacional del Control Mecanoquímico de Reacciones de Interés en Química Biorgánica.*
J. M. Bofill, I. de P. R. Moreira, Universitat de Barcelona
**CTQ2016-76423-P**, 2017-2019
Ministerio de Economía y Competitividad (MINECO)

*Understanding, controlling and optimizing heterogeneous catalysts and photocatalysts at the nanoscale. Application to carbon dioxide conversion and hydrogen production.*
F. Illas, S. T. Bromley, Universitat de Barcelona
**CTQ2015-64618-R**, 2016-2018
Ministerio de Economia y Competitividad (MINECO)

*Estructura electrónica y propiedades en moléculas y sólidos.*
E. Ruiz, Universitat de Barcelona
**CTQ2015-64579-C3-1-P**, 2016-2018
Ministerio de Economía y Competitividad (MINECO)

*Estructura electrónica y propiedades de moléculas y sólidos.*
P. Alemany, I. Díez-Pérez, Universitat de Barcelona
**CTQ2015-64579-C3-3-P**, 2016-2018
Ministerio de Economia y Competitividad (MINECO)

*Bioplastic Production From The Organic Fraction Of Municipal Solid Waste.*
J. Mata, J. Llorens, Universitat de Barcelona
**CTM2016-76275-R**, 2016-2019
Ministerio de Economia y Competitividad (MINECO)

*Modeling and Simulation of reactive processes in enzymes by means of ab initio molecular dynamics and QM/MM methods.*
C. Rovira, Universitat de Barcelona
**CTQ2017-85496-P**, 2018-2020
Ministerio de Economia y Competitividad (MINECO)

*Structure-based modeling of the role of the environment in photosynthetic light harvesting and protein fluorescence.*
C. Curutchet, Universitat de Barcelona
**CTQ2017-89924-P**, 2018-2020
Ministerio de Economia y Competitividad (MINECO)

*Diseño racional desde una perspectiva computacional de materiales basados en radicales orgánicos con propiedades de interés tecnológico.*
M. Deumal, J. J. Novoa, Universitat de Barcelona
**CTQ2017-87773-P**, 2018-2020
Ministerio de Economia y Competitividad (MINECO)

*Captura y separación de gases y contaminantes en procesos industriales sostenibles.*
R. Sayós, P. Gamallo, Universitat de Barcelona
**CTQ2014-53987-R**, 2015-2018
Ministerio de Economia y Competitividad (MINECO)

*Instituto Nacional de Bioinformática.*
M. Cascante, Universitat de Barcelona
**Ayudas para proyectos de investigación del área de Ciencias de la Salud (FIS),** 2018-2020
Ministerio de Economia y Competitividad (MINECO)

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

*FRAGments training NETwork (FRAGNET).*
X. Barril, Universitat de Barcelona
**675899**, 2016-2020
European H2020 Programme

*Identificación, síntesis y evaluación toxicológica de molécula propia antidetonante.*
F. J. Luque, R. Lavilla, J. Gómez, Universitat de Barcelona
Referència **309799,** 2018-2019
Contracto de arrendamientos y servicios de I+D con REPSOL, S.A.

*Computational modelling and molecular dynamics simulations of oil/water wettability on carbonate rocks and clays.*
R. Sayós, P. Gamallo, Universitat de Barcelona
2015-2018
Contracto de arrendamientos y servicios de I+D con REPSOL, S.A.

*Value added products for cosmetic from soybean by-product. Project DIOR-Barcelona.*
F. Mas, Universitat de Barcelona
Contracte amb empresa multinacional BUNGE IBÉRICA SAU, 2017-2018

*Estudi de laboratori i planta pilot per la recuperació d'amoni dels purins.*
F. Mas, Universitat de Barcelona
Contracte amb empresa multinacional INDUKERN (divisió veterinària), 2017-2019

*EXCIPHOCAT: - Tailoring the $TiO_2$ excited states by nanostructuring and hydroxylation: A step forward understanding photocatalytic water splitting.*
F. Illas, Universitat de Barcelona
**PRACE - 2016163940**, 2017-2018
Partnership for Advanced Computing in Europe (PRACE)

*Explicit Control Over Spin-States in Technology and Biochemistry.*
M. Swart, Universitat de Girona, C. Sousa, Universitat de Barcelona
**CM1305**, 2014-2018
European Framework for Cooperation in Science and Technology (COST)

*Knowledge Led Structure Prediction for Nanostructures.*
S. Woodley, University College London
**EP/K038958/1**, 2013-2018
Engineering and Physical Sciences Research Council (UK)

*Materials Networking.*
K. Neyman, Universitat de Barcelona
**European Commission, Ref. Nº 692146**, 2016-2019
European H2020 Cooperation Program - Research theme: 'Twinning' (H2020)

*Theoretical Chemistry and Computational Modelling.*
M. Yanez, Universidad Autonoma de Madrid
**TCCM-EJD**, 2014-2018
H2020 – ITN, Research and Innovation Framework Programme

*Theoretical Chemistry and Computational Modelling*
J. J. Novoa, Universidad Autonoma de Madrid
**TCCM-642294**, 2015-2018
Unió Europea (Marie Skłodowska-Curie Innovative Training Networks)

*A comprehensive and standardised e-infrastructure for analysing medical metabolic phenotype data (PhenoMeNal).*
M. Cascante, Universitat de Barcelona
**8P1ERI - H2020. PILLAR 1-EXCELLENT SCIENCE. ERI. European Research Infrastructures**.
**654241**, 2015-2018.
Unió Europea

*Theoretical Chemistry and Computational Modelling (TCCM).*
J. J. Novoa Vide, Universitat de Barcelona
**8P1MCA - H2020 PILLAR 1-EXCELLENT SCIENCE. MCA. Marie Sklodowska-Curie Actions**, 2015-2018.
Unió Europea

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

*Enhancing the scientific capacity of the Faculty of Chemistry and Pharmacy at Sofia University as leading regional research and innovation centre in the area of advanced functional materials (Materials Networking).*
K. Neyman, Universitat de Barcelona
**8SEWP - H2020. SEWP. Spreading Excellence and Widening Participation**, 2016-2019
Unió Europea

*QUIFIEXP - Química Física Experimental.*
J. Ignes, Universitat de Barcelona
**GINDO-UB/112**, 2016-2019
PPID - Projectes d'Innovació Docent (UB)

*NOMAD – Novel Materials Discovery.*
M. Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin
**NoMaD - 676580**, 2015-2018
H2020-EINFRA-5-2015, Centers of Excellence for Computing Applications

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

*Materiales nanoestructurados en catálisis: Análisis experimental de hallazgos obtenidos mediante modelización computacional.*
K. Neyman, Universitat of Barcelona
Universitat de Barcelona
**PRX17/00348**, 2018
Ministerio de Educación, Cultura y Deporte (MECD)

*Estudio del daño por radiación en materiales poliméricos mediante métodos de dinámica molecular cuántica no adiabática.*
P. Alemany, Universitat of Barcelona
Universitat de Barcelona
**PRX17/00268**, 2018
Ministerio de Educación, Cultura y Deporte (MECD)

*Mecanismos moleculares implicados en la inhibición de dianas para tratamientos anti-influenza: canal de protones M2 y hemaglutinina.*
F. J. Luque, Universitat de Barcelona
**SAF-2017-88107-R**, 2017-2020
Ministerio de Economia y Competitividad (MINECO)

*Discovery of New Antiparasitic Agents.*
F. J. Luque, Universitat de Barcelona, J. M. Bautista, Universidad Complutense de Madrid
2017-2018
Unión Iberoamericana de Universidades (UNIUN)

*Activadores de la proteína quinasa activada por AMP para el tratamiento de la enfermedad vascular asociada a la obesidad.*
F. J. Luque, Universitat de Barcelona, S. Fernández, A. Castro, Universidad Complutense de Madrid, CSIC
2018-2019
Fundació Eugenio Rodríguez Pascual

*Optimización de PharmScreen.*
F. J. Luque, E. Gibert, Universitat de Barcelona, Pharmacelera
2017-2018
Centro para el Desarrollo Tecnológico Industrial (CDTI)