Activity Report 2019

Grazynes: Carbon-Based Two-Dimensional Composites with Anisotropic Properties

The Journal of Physical Chemistry C
The creation of the Institute of Theoretical and Computational Chemistry of the *Universitat de Barcelona* (IQTCUB) was approved by the University’s Government Council in ordinary session in November 21st, 2007. From April 2018 I have the honour to serve as Director and I want to take the opportunity of being at the forefront of the IQTCUB’s annual memory for acknowledging explicitly to Dr. Jordi Poater for his participation in the previous IQTCUB’s direction team and also to Dr. Carles Curutchet for incorporating to the direction team. Additionally, from the point of view of external recognition the María de Maeztu awarding has allowed to incorporate new grant holders and postdocs to the Institute that give us an increase in the quality and quantity of our research. Another important point has been the incorporation of senior researchers through programs like Beatriu de Pinós, Juan de la Cierva, Ramón y Cajal and ICREA.

The common objective of the research projects developed in the Institute is the use of quantum chemistry methods, although recently with the inclusion of experimental groups from our departments new collaborations have started beyond Computational Chemistry fomenting and increasing the multidisciplinary character of our research. Traditionally, the IQTCUS’s research is different to that everyone expects for a traditional chemist, since the instrumentation used for our researchers is not found in a traditional laboratory but in a computational “laboratory” that usually is the entrance point to our resources or into supercomputing centres with computational capacity even higher.

The main objective of Theoretical and Computational Chemistry is to achieve the detailed understanding of chemical and physical processes for helping to interpret the experimental results and make predictions that lead to new experiments. According to that, this discipline can provide with new concepts that allow progressing in different aspects like the rational design of new materials with specific physical properties and in their application in electronics and magnetic devices; in the discovery of new medicines and in the understanding of the biochemical processes behind; in new reactions that improve the chemical processes for making them more effective and more environmentally-friendly; and in proposing new sustainable energy sources to overcome the challenges our society faces today. Moreover, we have to integrate in our research new tools like the automatic learning (artificial intelligence), virtual reality and new computational resources (“exascale” and quantum computation).

Eliseo Ruiz
Director of IQTCUB
I. IQTCUB OVERVIEW .......................................................... 3
I.1 Direction team 3
I.2 IQTCUB Research Lines 4
I.3 IQTCUB Members 5
I.4 Technical Staff 10
I.5 Equipment 10

II. IQTCUB ACTIVITIES 23
II.1 General Activities (courses, grants and dissemination) 23
II.2 IQTCUB Seminars and Conferences 31
II.3 IQTCUB Invited Researchers 34

III. SCIENTIFIC ACTIVITY OF IQTCUB MEMBERS 37
III.1 Highlights from most relevant results 37
III.2 Publication list 55
   Published articles 55
   Book chapters and proceedings 69
III.3 Other activities 70
   Doctoral Theses 70
   Masters Theses 72
   Scientific Conferences and Meetings 76
   Research Stays in Recognized Centers 96
   Participation in Competitive Funded Research Projects 97
I. IQTCUB OVERVIEW

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

I.1 DIRECTION TEAM

The IQTCUB direction team during 2019 has been,

Prof. Eliseo Ruiz Sabin  Director
Prof. Carles Curutchet Barat  Secretary (Sept-Dec)
Prof. Jordi Poater Teixidor  Secretary (Jan-Sept)
Prof. Francesc Illas Riera  Board member
1.2 IQTCUB Research Lines

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

1. Clean and sustainable energy

   What are the mechanisms of crucial chemical processes in energy conversion? Computational chemistry modelling can help in the design of new catalytic materials that can be crucial for electricity production in fuel-cell systems, as well as the catalysts involved in the activation of CO\textsubscript{2} and chemical or electrochemical conversion into useful molecules such as methane, ethylene or ethanol. Furthermore, theoretical approaches could also provide valuable insights into the mechanisms of the oil-water-rock interactions involved in the enhancement of oil recovery.

2. Nanomaterials and nanoelectronics

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

3. Biomedicine and Soft Matter

   What are the key molecular mechanisms in biological systems? Simulations involving thousands of atoms can be applied to model biomaterials and molecular mechanisms in biologically relevant molecules. Theoretical approach and the implementation of quantum chemistry and mechanical chemistry is useful to investigate the structure and reactivity of proteins and enzymes, to design new drugs, to describe processes in cellular membranes, enzymatic reactions in crowded media and soft nanoparticles in solution.
I.3 IQTCUB Members

IQTCUB involves a total of 101 professors and researchers: The full list of members of IQTCUB (including the corresponding academic situation and affiliation within UB) is provided below.

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## Other Categories (Professors Agregats)

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## ICREA Research Professors

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## Other Categories (Professors Associats)

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**Postdoctoral contracts**

**Beatriu de Pinós-Juan de la Cierva**

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**Ramón y Cajal**

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**Contracte Projecte de Recerca**

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**Ph.D. Students**

**Beca Programa María de Maeztu**

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**FI Grant (Catalan Government Program)**

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

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**Beca CONICYT**

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### I. IQTCUB Overview

#### Beca Doctorat Industrial

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<td>Vila Julià</td>
<td>Guillem</td>
<td>M</td>
<td>Materials Science &amp; Physical Chemistry</td>
</tr>
</tbody>
</table>

---

Distribution of IQTCUB members according to the professional category.

- **Full Profs.**
- **Associate Prof.**
- **Prof. Agregats**
- **Prof. Associates**
- **Prof. Lectors**
- **ICREA Res.**
- **Postdoc Res.**
- **Ph.D. students**
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 €)

<table>
<thead>
<tr>
<th>Machine type</th>
<th>SUN cluster (4 racks)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Operating system</td>
<td>SLES10</td>
</tr>
<tr>
<td>Services</td>
<td>Calculation cluster and disk server (raid of 2.5TB). Internal DHCP server</td>
</tr>
<tr>
<td>Structure</td>
<td>Master + 111 nodes</td>
</tr>
<tr>
<td>Notes</td>
<td>There are heterogeneous nodes with 32 and 64 bits processors.</td>
</tr>
</tbody>
</table>
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)
### IQTCUB Overview

#### IQTC01 (invested value 250,000 €)

<table>
<thead>
<tr>
<th><strong>Machine type</strong></th>
<th>HP cluster</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Operating system</strong></td>
<td>Debian Stable</td>
</tr>
<tr>
<td><strong>Services</strong></td>
<td>Calculation cluster</td>
</tr>
<tr>
<td><strong>Structure</strong></td>
<td>80 nodes</td>
</tr>
<tr>
<td><strong>Notes</strong></td>
<td>64 bits processors</td>
</tr>
</tbody>
</table>

**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 €)

<table>
<thead>
<tr>
<th><strong>Machine type</strong></th>
<th>HP cluster</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Operating System</strong></td>
<td>SLES10</td>
</tr>
<tr>
<td><strong>Services</strong></td>
<td>Calculation cluster</td>
</tr>
<tr>
<td><strong>Structure</strong></td>
<td>26 nodes</td>
</tr>
<tr>
<td><strong>Notes</strong></td>
<td>64 bits processors</td>
</tr>
</tbody>
</table>

**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 €)**

<table>
<thead>
<tr>
<th>Machine type</th>
<th>SGI Cluster</th>
</tr>
</thead>
<tbody>
<tr>
<td>Operating System</td>
<td>SLES11</td>
</tr>
<tr>
<td>Services</td>
<td>Calculation cluster</td>
</tr>
<tr>
<td>Structure</td>
<td>4 nodes</td>
</tr>
<tr>
<td>Notes</td>
<td>64 bits processors</td>
</tr>
</tbody>
</table>

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)
I. IQTCUB OVERVIEW

**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 10 gigabit 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 10 gigabit network card (internal data network)
**I. IQTCUB Overview**

**iqtc08 (invested value 175,000 €)**

*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 75,000 €)**

*Machine type*  
Heterogeneous Cluster

*Operating System*  
SLES11, centos 7

*Services*  
Calculation cluster with GPUs

*Structure*  
5 nodes

*Notes*  
64 bits processors

**Specifications:**

**Node**

CPU: 1 x 3.06 GHz Intel Core i7 950  
RAM: 16 GB  
HD: 1 x 1 TB hard disk  
Network: 1 gigabit network card (calculation network)  
GPU: 1 NVIDIA GTX580, 1 NVIDIA GTX480

**Node Tyan FT72B7015**

CPU: 2 x 2.66 GHz Xeon SixCore  
RAM: 48 GB  
HD: 1 x 500 GB hard disk  
Network: 4 gigabit network card (calculation network) + 1 IPMI card (OOB)  
GPU: 8 NVIDIA GTX580
Node
CPU: 1 x 3.30 GHz AMD FX-4100 QuadCore
RAM: 16 GB
HD: 1 x 1 TB hard disk
Network: 1 gigabit network card (calculation network)
GPU: 1 NVIDIA GTX770

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

Node ASUS ESC4000 G2
CPU: 2 x 2.4 GHz Xeon SixCore
RAM: 32 GB
HD: 1 x 1 TB hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (OOB)
GPU: 4 NVIDIA GTX TITAN BLACK

Node AZServer 4G3S
CPU: 2 x 2.4 GHz Xeon E5-2620v3
RAM: 32 GB
HD: 1 x 1 TB hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (OOB)
GPU: 4 NVIDIA GTX 980

Node SIE LADON BROADWELL
CPU: 2 x 2.4 GHz Xeon E5-2640v4
RAM: 128 GB
HD: 1 x 1 TB hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (OOB)
GPU: 4 NVIDIA TESLA K40

Node SIE LADON BROADWELL 2
CPU: 2 x 2.4 GHz Xeon E5-2640v4
RAM: 128 GB
HD: 1 x 1 TB hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (OOB)
GPU: 2 NVIDIA TESLA P100
2 Nodes AZServer 4G3S
CPU: 2 x 2.2 GHz Dual Xeon E5-2600v4 (10 cores)
RAM: 128 GB
HD: 2 x 2 TB hard disk
Network: 4 gigabit network card + 1 IPMI card (OOB)
GPU: 4 NVIDIA GEFORCE GTX 1070Ti

SERVERS

Glusterfs disk server (invested value 54.000 €)
Machine type DELL cluster
Operating system SLES 11
Services Storage service cluster with 8TB of space for applications directories and user’s work area exported by GlusterFS
Structure 2 nodes
Notes Storage service with a dedicated UPS and redundant power supply
Specifications:

2 INTEL DELL PowerEdge 2950 nodes
CPU: 2 x 2.50 GHz Xeon QuadCore E5420
RAM: 8 GB
HD: 4 x 1 TB (raid 5)
Network: 2 gigabit network card (internal network)

Machine type HP cluster
Operating system SLES 11
Services Storage service cluster with 32TB of space for user’s data exported by GlusterFS
Structure 2 nodes
Notes Storage service with a dedicated UPS and redundant power supply
Specifications:

1 INTEL HP ProLiant DL180 G6 node
CPU: 2 x 2.27 GHz Xeon QuadCore E5520
RAM: 56 GB
HD: 12 x 2 TB (raid 5)
Network: 2 gigabit network card (internal network) + 1 IPMI card (OOB)
1 INTEL HP ProLiant DL380e Gen8 node
CPU: 2 x 2.20 GHz Xeon QuadCore E5-2407
RAM: 48 GB
HD: 12 x 2 TB (raid 5)
Network: 2 gigabit network card (internal network) + 1 IPMI card (OOB)

Machine type: Supermicro
Operating system: Centos 7.6

Services: Storage service cluster with 64TB of space for applications directories and user's work area exported by NFS
Structure: 1 node
Notes: Storage service redundant power supply

Specifications:

1 Node Supermicro 2U
CPU: 2 x 2.20 GHz Xeon 4210
RAM: 64 GB
HD: 8 x 8 TB (raid 5)
Network: 4 gigabit network card
Network: 2 10GB network card

Machine type: DELL
Operating system: Centos 7.6
Services: Storage service cluster with 100TB of space for applications directories and user's work area exported by GlusterFS
Structure: 1 node
Notes: Storage service redundant power supply
Specifications:

1 PowerEdge R740XD
CPU: 2 x 2.10 GHz Xeon 4110
RAM: 64 GB
HD: 10 x 10 TB (raid 5)
Network: 4 gigabit network card
Network: 2 10GB network card

Portal (user access servers) (invested value 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
## I. IQTCUB Overview

### 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 28.300 €)*

<table>
<thead>
<tr>
<th>Machine type</th>
<th>4 redundant nodes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Operating system</td>
<td>Debian stable</td>
</tr>
<tr>
<td>Services</td>
<td>Xen, DRBD, IQTCUB internal services</td>
</tr>
<tr>
<td>Structure</td>
<td>4 redundant nodes</td>
</tr>
<tr>
<td>Notes</td>
<td>Servers that contains the Xen virtual machines with the IQTCUB's internal services (SGE, dhcp, license server, etc.). Critical service connected with a UPS</td>
</tr>
</tbody>
</table>

### 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)

<table>
<thead>
<tr>
<th>Machine type</th>
<th>1 node</th>
</tr>
</thead>
<tbody>
<tr>
<td>Operating system</td>
<td>Centos 7.3</td>
</tr>
<tr>
<td>Services</td>
<td>Pre-production and testing proposals</td>
</tr>
<tr>
<td>Structure</td>
<td>1 node</td>
</tr>
</tbody>
</table>

### Specifications:

**1 DELL PowerEdge R640**  
CPU: 2 x 2 GHz Xeon Gold 6138  
RAM: 128 GB  
HD: 2 x 2 TB (raid 1)  
Network: 2 gigabit network card + iDrac
I. I Q T C U B  O V E R V I E W

Graphical applications server *(invested value 3.000 €)*

<table>
<thead>
<tr>
<th><strong>Machine type</strong></th>
<th>1 HP ProLiant DL385 node</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Operating system</strong></td>
<td>Debian Stable</td>
</tr>
<tr>
<td><strong>Services</strong></td>
<td>Server for the use of graphical applications (gaussview, p4vasp, etc.)</td>
</tr>
<tr>
<td><strong>Structure</strong></td>
<td>1 node</td>
</tr>
<tr>
<td><strong>Notes</strong></td>
<td>Server connected to an UPS</td>
</tr>
</tbody>
</table>

**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 I Q T C U B have other services to provide service to the I Q T C U B'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 I Q T C U B's network).
5. Switch Layer 3 HP Procurve with 24 ports (used for the I Q T C U B's date centre infrastructure).
6. 8 Switchs Layer 2 Dlink with 48 ports (internal network for cerq12, iqtco1, iqtc02, iqtc03 clusters).
7. 4 Switchs Layer 2 HP with 48 ports (internal network for iqtc04, iqtc05 and iqtc06 cluster).
I. IQTCUB OVERVIEW

8. 3 Switchs Infiniband Voltaire with 36 ports (calculation network for iqtc04 cluster).

9. Modular switch HP (8 calculation network modules for iqtc01, iqtc02, iqtc03 clusters).

10. 2 Modular switch HP 10GB (calculation network for iqtc06 and data network for the glusterfs servers).

11. 2 Switch Netgear XS728T 10GB (internal and calculation network for iqtc08).

12. 1 Switch HPE 1810-24 (internal network iqtc08).

13. 1 MSI LAPTOP with Oculus RIFT S -Virtual Reality Study-.

The approximated invested cost of this equipment is 53.000 €.

SUMMARY

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Cores</td>
<td>4,062 c</td>
</tr>
<tr>
<td>Memory</td>
<td>38,886 GB RAM</td>
</tr>
<tr>
<td>Calculation disk capacity</td>
<td>266 TB</td>
</tr>
<tr>
<td>Data user disk capacity</td>
<td>132 TB</td>
</tr>
</tbody>
</table>

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

2.100.000 €*

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

II.1 GENERAL ACTIVITIES

Next, a description of activities and actions promoted by IQTCUB through 2019 is provided.

a. **Promotion and encouragement of research.** This year the IQTCUB has finally offered one 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 Silvia Sodric for starting Master studies under the supervision of Dr. Jordi Poater.

*Total cost: 2.680 €*
b. **10th IQTCUB workshop.** This one-day workshop aimed at the dissemination of the research done at the IQTCUB took place on May 31st, 2019 at it was organized by Dr. Jordi Cirera. The IQTCUB members and internationally acknowledged speakers present the most recent work. This year we highlight the participation of Prof. Dr. Martin Kaupp from the Technische Universität Berlin with the invited lecture entitled *New Quantum Methods and New Applications: NMR/EPR Parameters, Local Hybrid Functionals, and more,* and Prof. Dr. John E. McGrady from the University of Oxford with the invited lecture entitled *Pushing molecules around: a theoretical perspective on the chemical bond, and how to modify it.* The other invited speakers were Dr. Axel Bidon-Chanal (*Computational biology and gastronomy research in the food and nutrition Torribera campus*), Joan Coines (*Mechanistic insights into substrate-assisted glycoside hydrolases*) and Antoni Macià (*A computational view on astronomical silicate nanoclusters*) all three from University of Barcelona and IQTCUB. Moreover, 17 poster contributions have been presented during the meeting (https://www.iqtc.ub.edu/news/posters-at-the-iqtcub-symposium-2019/). The IQTCUB assigned a budget to cover the traveling and lodging expenses of the invited professors as well as the catering service offered to all assistants.

Total cost: 1.491 € + 2.000 € economic assignment of Faculty of Chemistry
c. **IQTC Scientific Advisory Board Meeting.** On November 29th 2019 it was held the first IQTCUB scientific advisory meeting with the participation of Profs. Agustí Lledós (Universitat Autònoma de Barcelona), John McGrady (University of Oxford), Sofía Calero (Universidad Pablo de Olavide), Federico Gago (Universidad de Alcalà), Carmen Domene (University of Bath) i Roser Valentí (Goethe-Universität Frankfurt).

*Total cost: 3,650 €*
II. IQTCUB Activities

_df_. **Scientific Dissemination Activities.** Prof. Xavier Giménez Font has been involved in the following scientific and teaching dissemination activities during 2019:

II. IQTCUB Activities

34. “UB s’Apropa 19”. INS Torres i Bages, Hospital de Llobregat, 20/Mar/2019.
II. IQTCUB ACTIVITIES

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

   https://elpais.com/cultura/2019/01/04/actualidad/1546601992_837620.html

2. “La Màgia de l’Aigua”, Conference within the series “Pessics de Ciència”, Centre Cultural Sant Josep.
   L’Hospitalet de Llobregat, March 27th, 2019.
   https://www.youtube.com/watch?v=3oRJf6LEVug&feature=youtu.be

3. “SABER: Let’s make high students performance possible, even in STEM courses”, METID & Faculty seminar.
   https://www.youtube.com/watch?v=gljsJ1uYPm0&feature=youtu.be

   https://www.lavanguardia.com/comer/tendencias/20190627/463134511552/enfriar-bebidas-ola-de-calor-refrescos-velocidad-rapido.html?fbclid=IwAR26NWDDnwllDxdyTpgPdyx7labLYNCdTaFJqy5CgKBl5u87TCJwdcweh0I


7. “Què són les bateries d’ió-liti, el motiu del Premi Nobel de Química d’enguany”, interviewed by Sandra Mestres, betevé notícies vespre program, Betevé Televisió, Barcelona, October 11th, 2019
https://beteve.cat/btv-noticies-vespre/btv-noticies-vespre-1388/

8. “Els filtres de partícules als motors diésel”, interviewed by Xavier Muixí, Betevé Notícies Vespre program, Betevé Televisió, Barcelona, November 27th, 2019
https://beteve.cat/btv-noticies-vespre/btv-noticies-vespre-1427/

Other dissemination activities carried out for IQTC members during 2019 are the following:

1. “Fem Química al Laboratori”

2. “V Festa de la Ciència de la UB”
   http://www.ub.edu/laubdivulga/festacienciaub/festacienciaV/index.html
II.2 IQTCUB SEMINARS AND CONFERENCES

During 2019 Dr. Jordi Poater has organized the following IQCT’s seminars and conferences:

1. **Dr. Maytal Caspary** (Israel Institute of Technology), Haifa, Israel.  
   *Recent advances in modeling Fe$_2$O$_3$ for water splitting catalysis*  

2. **Dr. Umberto Terranova** (University of Cardiff) Cardiff, United Kingdom.  
   *Iron sulphide minerals: phase stability and oxidation behavior*  
   8 February 2019.

3. **Dr. Alejandro Rodríguez** (Int. Center of Theoretical Physics), Trieste, Italy.  
   *The fuzzy border between Molecular Simulations and data science*  
   5 March 2019.

4. **Dr. Mercedes Alfonso** (IAS-5, INM-9), Jülich, Germany.  
   *Understanding ligand selectivity in bitter taste receptors using multiscale molecular dynamics simulations*  
   22 March 2019.

5. **Prof. Aliaksandr Bandarenka** (Technische Universität München), Munich, Germany.  
   *Why electrolytes control the catalytic activity*  
   8 April 2019.

6. **Dr. Taehum Lee** (Yonsei University), Seoul, South Korea.  
   *Characterization of ultrathin oxidic metal layers on another surrogate metal support: A theoretical surface science approach*  
   9 April 2019.
II. IQTCUB ACTIVITIES

7. **Dr. Julian Gebhardt** (Max Planck Institute), Hamburg, Germany.
   *New Materials from Simulations*
   26 April 2019.

8. **Prof. Anela Ivanova** (Sofia University), Sofia, Bulgaria.
   *Molecular design of new organic TADF emitters*
   3 May 2019.

9. **Prof. Vladimir Guterman** (Southern Federal University), Rostov-on-Don, Russia.
   *Pt-Containing Nanostructured Electrocatalysts for Low-Temperature Fuel Cells*
   21 May 2019.

10. **Prof. Francisco Zaera** (University of California), Riverside, USA.
    *The Route to Better Catalysts: From Surface Science to Nanotechnology*
    24 May 2019.

11. **Prof. Diana Cheshmedzhieva** (University of Sofia), Sofia, Bulgaria.
    *Application of theoretical computations in studying reaction mechanisms and reactivity of organic compounds*
    18 June 2019.

12. **Dr. Isaac Alcón** (Freie Universität Berlin), Berlin, Germany.
    *Quantum interference engineering of nanoporous graphene for carbon nanocircuitry*
    8 October 2019.

13. **Dr. Sergi Vela** (EPFL), Lausanne, Switzerland and (Université Strasbourg) Strasbourg, France.
    *Modern Computational Tools to Investigate Spin Crossover and Azoheteroarene-based molecular switches*
    21 October 2019.
14. **Prof. Notker Rösch** (Technische Universität München), Munich, Germany.
   *Single Atom Catalysis – a Theoretician’s Dream Scenario? Lessons from Working on C-C Coupling over Zeolite-supported Rh(I)*
   6 November 2019.

15. **Dr. Aleix Comas-Vives** (Universitat Autònoma de Barcelona), Bellaterra, Spain.
   *Ab Initio and Multiscale Modelling of CO₂ Conversion to Methanol and Syngas: Active Sites and Selectivity*
   11 December 2019.
II. IQTCUB ACTIVITIES

II.3 IQTCUB INVITED RESEARCHERS

During 2019, a total of twenty-two researchers have spent some time at the IQTCUB collaborating in different research projects.

1. **Prof. Hristiyan Aleksandrov** (invited researcher).
   University of Sofia, Bulgaria.

2. **Prof. Iskra Koleva** (invited researcher).
   University of Sofia, Bulgaria.

3. **Dr. Annika Borg** (invited researcher).
   Graz University of Technology, Austria.
   February 2019.

4. **Dr. David Gobrecht** (HPC Europa researcher)
   Katholieke Universiteit Leuven, Belgium.
   February 2019.

5. **Dr. Juan Aragó** (invited researcher).
   Institut de Ciència Molecular de la Universitat de València, Spain.
   March 2019.

6. **MSc. Laura Granda** (HPC Europa researcher)
   Leiden University, Netherlands.
   April-july 2019.

7. **Dr. Ciro Achille** (invited researcher).
   University of Pàdova, Italy.
   May 2019.
8. Prof. Anela Ivanova (invited researcher).
   University of Sofia, Bulgaria.
   May 2019.

   University of Sofia, Bulgaria.
   June 2019.

10. Prof. Rositca Nikolova (invited researcher).
    University of Sofia, Bulgaria.
    June 2019.

11. Dr. Miroslava Nedyalkova (invited researcher).
    University of Sofia, Bulgaria.
    June-july 2019.

12. Prof. Vasil Simeonov (invited researcher).
    University of Sofia, Bulgaria.
    July 2019.

13. Dr. Rita Dias (invited researcher).
    NTNU, Norway.
    October 2019.
    July 2019.

14. Dr. Lorenzo Mino (invited researcher).
    Università degli Studi di Torino, Italy.
    July-august 2019.
15. **MSc. Cameron Beevers** (HPC Europa researcher).
   Cardiff University, United Kingdom.
   September-november 2019.

16. **Antonio Pantoja** (invited researcher).
    UNAM, Mexico.

17. **MSc. Hedda Oschinski** (ERASMUS researcher).
    Leibniz University, Germany.

18. **Dr. Enrico Bisquoli** (invited researcher).
    University of Pisa, Italy.
    October-december 2019.

19. **Dr. Ludivine Levedel** (invited researcher).
    University of Poitiers, France.
    November 2019.

20. **Prof. Maria Hrmova** (invited researcher).
    University of Adelaide, Australia.
    November 2019.

21. **Dr. Giovanni Di Liberto** (HPC Europa researcher).
    Università degli Studi di Milano-Bicocca, Italy.
    November-december 2019.

22. **Dr. Massomeh Keyhanian** (invited researcher).
    University of Mazandaran, Iran.
III. SCIENTIFIC ACTIVITY OF IQTCUB MEMBERS

III.1 HIGHLIGHTS FROM MOST RELEVANT RESULTS

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

LINE 1. CLEAN AND SUSTAINABLE ENERGY

Using density functional calculations to elucidate atomic ordering of Pd-Rh nanoparticles at sizes relevant for catalytic applications.

L. Vega, H. A. Aleksandrov, K. M. Neyman.


DFT modelling identifies surface composition of Pd-Rh particles of thousands atoms and paves the way for evaluating surface segregation due to adsorbed reactants.

This study quantifies, with the help of density functional (DFT) calculations and our novel Topological Approach, atomic ordering and surface segregation effects in Pd-Rh particles with compositions 1:3, 1:1 and 3:1 containing up to 201 atoms (ca. 1.7 nm). The obtained data are used to reliably optimise energetically preferred atomic orderings in inaccessible by DFT Pd-Rh particles containing thousands of atoms and exhibiting sizes exceeding 5 nm, which are typical for catalytic metal particles. It is outlined, how segregation effects on the surface arrangement of Pd-Rh nanoalloy catalysts induced by adsorbates can be evaluated in a simple way within the present modelling setup.
Kinetic Monte Carlo simulations unveil synergic effects at work on bifunctional catalysts.


The interaction between metal particles and the support in heterogeneous catalysis has been the subject of a large number of studies. While strong metal–support interactions can lead to deleterious catalyst deactivation and the underlying mechanism is well understood, in other cases the effect may beneficially enhance the catalytic activity and/or selectivity with no clear picture of the chemistry involved. The kMC simulations provide strong evidence for a cooperative effect between the different regions of the catalyst Au/MoC. Thus, the clean MoC regions are responsible for adsorbing and dissociating water molecules, and the vicinity of the Au adclusters contributes to COOH formation.
Pressure selection for non-reactive and reactive pressure-swing distillation.


Theoretical study of simulation that shows that when the heating services increase their quality, i.e. low, medium or high pressure steam, their costs increase suddenly. This point must be considered when optimizing the pressure of a pressure swing distillation.
Ion-pair formation in neutral potassium-neutral pyrimidine collisions: electron transfer experiments.

A. M. Mendes; B. Pamplona, S. Kumar; F. Ferreira da Silva, A. Aguilar, G. García, M. C. Bacchus_Montabonel, P. Limao-Vieira.


![Graph showing branching ratios for different ions](image)

Pyrimidine branching ratios (fragment anion yield/total anion yield) of the main negative ions formed as a function of the collision energy in the center-of-mass frame.

We report on ion-pair formation in hyperthermal (30–800 eV) neutral potassium collisions with neutral pyrimidine molecules. Negative ions formed by electron transfer from the alkali atom to the target molecule were time-of-flight mass analysed and the fragmentation patterns and branching ratios obtained. The most abundant product anions have been assigned to CN$^-$ and C$_2$H$^-$ and the electron transfer mechanisms are comprehensively discussed. Theoretical calculations were performed for pyrimidine in the presence of a potassium atom and provided a strong basis for the assignment of the lowest unoccupied molecular orbitals accessed in the collision process. In order to further our knowledge about the collision dynamics, potassium cation (K$^+$) energy loss spectrum has been obtained and within this context, we also discuss the role of the accessible electronic states. A vertical electron affinity of (-5.69 ± 0.20) eV was obtained and may be assigned to a π*$_3$(b$_1$) state that leads to CN$^-$ formation.
The gas phase oxidation of HCOOH by Cl and NH$_2$ radicals. Proton coupled electron transfer versus hydrogen atom transfer.

J. M. Anglada, R. Crehuet, A. Solé.


Examples of hat and pcet reaction mechanisms.

The reaction of formic acid (HCOOH) with chlorine atom and amidogen radical (NH$_2$) have been investigated using high level theoretical methods such BH&HLYP, MP2, QCISD, and CCSD(T) with the 6–311+G(2df,2p), aug-cc-pVTZ, aug-cc-pVQZ and extrapolation to CBS basis sets. The abstraction of the acidic and formyl hydrogen atoms of the acid by the two radicals has been considered, and the different reactions proceed either by a proton coupled electron transfer (pcet) and hydrogen atom transfer (hat) mechanisms. Our calculated rate constant at 298 K for the reaction with Cl is $1.14 \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ in good agreement with the experimental value $1.8\pm0.12/2.0 \times 10^{-13}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ and the reaction proceeds exclusively by abstraction of the formyl hydrogen atom, via hat mechanism, producing HOCO+ClH. The calculated rate constant, at 298 K, for the reaction with NH$_2$ is $1.71 \times 10^{-15}$ cm$^3$ molecule$^{-1}$ s$^{-1}$, and the reaction goes through the abstraction of the acidic hydrogen atom, via a pcet mechanism, leading to the formation of HCOO+NH$_3$. 
Rotational energy relaxation quantum dynamics of a diatomic molecule in a superfluid helium nanodroplet and study of the hydrogen isotopes case.

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


Populations of the \((j=0, m_j=0)\) (solid lines) and \((j=2, m_j=0)\) (dashed lines) rotational states of molecules, as a function of time.

The rotational energy relaxation (RER) of a molecule \(X_2(j, m_j)\) in a \(^4\)He superfluid nanodroplet [HeND; \(T=0.37\) K] was studied using a hybrid quantum dynamics approach proposed by us. This is the first theoretical study about RER in HeNDs and here several isotopes of \(H_2\) were examined. The structure of the HeND does not change during the RER, which takes place according to a cascade mechanism and \(m_j\) is conserved. The lifetime of an excited rotational state (\(\approx 1.0-7.6\) ns) increases when \(B_0\) increases, \(j\) increases, and \(N\) decreases (above \(N=100\) He atoms there is a small influence of \(N\) on the lifetime). The analysis of the influence of the coupling between the \(j - j\)-2 rotational states and the \(X_2\) angular velocity on the lifetime was helpful to interpret the results. We hope that the present study will encourage more studies on RER in HeND, a basic, interesting and difficult to study phenomenon about which we still know very little.
Grazynes: carbon-based two-dimensional composites with anisotropic properties.
S. Kamalinahad, F. Viñes, P. Gamallo.


A new family of two-dimensional carbon allotropes is presented, based on graphene stripes linked to each other by acetylenic connections. The large amount of allowed connectivities demands a family name for them: grazynes. The present study reports the energetic, structural, elastic, and electronic physicochemical properties of a set of simple grazynes by means of density-functional-theory-based calculations, suggesting also possible synthetic routes. The main results conclude that these are exotic yet stable materials, stiffer than graphene in the acetylenic direction, highly anisotropic, and with the presence of Dirac points in the reciprocal space along the graphene stripes direction resistant to strain, regardless of its direction. Thus, grazynes infer directionality in electron conductivity and resilience to the material stretching/compression, quite important, for instance, in the nanoelectronics applicability point of view.
LINE 2. NANOMATERIALS AND NANOELECTRONICS

Interplay between the gentlest ascent dynamics method and conjugate directions to locate transition states.


![Image](image.png)

Behaviour of the curve GAD-CD (blue) on a PES. The set of arrows (green) shows the evolution of the control vectors.

An algorithm to locate transition states on a potential energy surface (PES) was proposed and described. The technique is based on the gentlest-ascent-dynamics (GAD) method where the gradient of the PES is projected into a given direction and also perpendicular to it. In the proposed method, named GAD-conjugate-direction (GAD-CD), the projection is not only applied to the gradient but also to the Hessian matrix. Then, the resulting Hessian matrix is block diagonal. The direction is updated according to the GAD method. Furthermore, to ensure stability and to avoid a high computational cost, a trust region technique is incorporated and the Hessian matrix is updated at each iteration. The performance of the algorithm in comparison with the standard ascent dynamics is discussed for a simple two-dimensional model PES. Its efficiency for describing the reaction mechanisms involving small and medium size molecular systems is demonstrated for molecular systems of interest in chemistry.
Deactivation of excited states in transition metal complexes: Insight from computational chemistry.


Investigation of the excited state decay dynamics of transition-metal systems is a crucial step for the development of photoswitchable molecular based materials with applications in growing fields as energy conversion, data storage, or molecular devices. An overview is presented of the state-of-the-art methodologies available to address the several aspects that have to be incorporated to properly describe the deactivation of excited states in transition-metal complexes.
Reorganization of intermolecular interactions in the polymorphic phase transition of a prototypical dithiazolyl-based bistable material.


The spin transitions undergone by several molecular crystals of dithiazolyl (DTA) radicals make this type of radical promising candidates for future sensors and memory devices. In this work, we performed a systematic computational study of the intermolecular interactions existing in the two polymorphs of the neutral radical 1,3,5-trithia-2,4,6-triazapentalenyl in order to elucidate the origin of the difference in energy between those two polymorphs involved in its spin transition and to understand the crystal packing of this prototype of bistable materials. The π−π interactions between radicals are the main driving force for the crystal packing of both polymorphs, which comprises π-stacks of radicals. The difference in energy between polymorphs, in turn, is mainly controlled also by the intrastack π−π intermolecular interactions, and the interstack S⋯S contacts. Since the supramolecular motifs herein identified as important for the crystal packing and/or for the energy difference between polymorphs (and, thus, for the spin transition temperature) are common to other members of the DTA family, our results provide valuable information to understand better the structure and properties of other switchable DTA-based materials.
Structure and properties of nanosilicates with olivine \((\text{Mg}_2\text{SiO}_4)_n\) and pyroxene \((\text{MgSiO}_3)_n\) compositions.


Magnesium-rich silicates are ubiquitous both terrestrially and astronomically, where they are often present as small particles. Nanosized Mg-rich silicate particles are likely to be particularly important for understanding the formation, processing, and properties of cosmic dust grains. Overall, our work provides a new platform for an accurate and detailed understanding of nanoscale silicates.
Effects of temperature on the shape and symmetry of molecules and solids.

How does temperature change the shape of molecules? Bridging the gaps between Plato and Boltzman using continuous shape measures.

Despite its undeniable problems from a philosophical point of view, the concept of molecular structure, with attributes such as shape and symmetry, directly borrowed from the description of macroscopic objects, is nowadays central to most of chemistry. Following this trend, descriptions such as "the tetrahedral" carbon atom are widely used from elementary textbooks to the most up-to-date research articles. The definition of molecular shape is, however, not as simple as it might seem at first sight. Molecules don't behave as macroscopic objects do due to the incessant motion of its constituent particles, nuclei and electrons. How are molecular shape and symmetry affected by this thermal motion? In this review we introduce the language of continuous symmetry measures as a new tool to quantitatively describe the effects of temperature on molecular shape and symmetry.
[UF₆]²⁻: A molecular hexafluorido actinide(IV) complex with compensating spin and orbital magnetic moments.


Cartoon that symbolizes the combination of computational and experimental studies on a novel uranium anion.

Synthesis, structural determination and spectroscopic and magnetic studies of a novel uranium anion, carried out by an international team in which two researchers from the IQTC were in charge of the multireference CASSCF calculations that allow to explain the unexpectedly very small magnetization found in synchrotron XMCD (X-ray magnetic circular dichroism) measurements as due to the compensation of spin and orbital contributions.
**III. SCIENTIFIC ACTIVITY OF IQTCUB MEMBERS**

**LINE 3. BIOMEDICINE AND SOFT MATTER**

Spectral variability in phycocyanin cryptophyte antenna complexes is controlled by changes in the α polypeptide chains.


Multiscale simulations indicate that differences in the light harvesting properties of the PC577, PC612, PC630 and PC645 cryptophyte antenna complexes arise from changes in the α polypeptide chains in the structure.

Quantitative models of light harvesting in photosynthetic antenna complexes depend sensitively on the challenging determination of the relative site energies of the pigments. This study analyzed the basis of the light harvesting properties of four antennae from cryptophyte algae (PC577, PC612, PC630 and PC645), which have attracted much attention due to the recent observation of coherence effects in their light-harvesting mechanisms. By using multiscale polarizable quantum/molecular mechanics (QM/MMPol) calculations, it demonstrates that these four proteins share a common energetic ordering PCB82 < PCB158 < DBV51/61 for pigments located in the highly-conserved β chains, whereas bilins in the more divergent α chains cause their spectral differences. Moreover, the study provides a solid excitonic Hamiltonian of these proteins that paves the way for a detailed analysis of the basis supporting the coherence effects observed in their energy transport processes.
We report a versatile strategy to derive a pH-adapted scale that relies on theoretical estimates of distribution coefficients from conformational ensembles of amino acids. This is accomplished by using an accurately parametrized version of the IEFPCM/MST continuum solvation model as an effective way to describe the partitioning between n-octanol and water, in conjunction with a formalism that combines partition coefficients of neutral and ionic species of residues and the corresponding pKa values of ionizable groups. Two weighting schemes are considered to derive solvent-like and protein-like scales, which have been calibrated by comparison with other experimental scales developed in different chemical/biological environments and pH conditions as well as by examining properties such as the retention time of small peptides and the recognition of antigenic peptides. A straightforward extension to nonstandard residues is enabled by this efficient methodological strategy.
Deciphering the enzymatic mechanism of sugar ring contraction in UDP-apiose biosynthesis.


In changing weather situations, plants need to be robust and flexible at the same time. These structural properties are anchored the cell walls, which are largely built from polymers and polysaccharides. As binding agents, polysaccharides have the important task to connect long-chain polymers and to build a molecular network of tiny strands, called fibrils, which contribute to the tensile strength of the plant. One of the sugar building blocks is the branched-chain monosaccharide apiose. The mechanism responsible for apiose production of in nature was still unknown. Recently it has been discovered how apiose is produced by a single enzyme called UAXS (UDP-apiose/UDP-xylose Synthase) and the entire mechanism of this enzyme has been decoded by an interdisciplinary collaboration. The UAXS-enzyme selectively catalyzes four reaction steps, resulting in the change from a six ring sugar molecule (hexose) to a structural converted five ring sugar (pentose). By creating new organic carbon compounds, the enzyme is responsible for giving plants their strength properties.
Effect of charge regulation and conformational equilibria in the stretching properties of weak polyelectrolytes.

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


Schematic of a weak polyelectrolyte model under the influence of pH, ionic strength and external force. Monomers are represented as sites joined by flexible harmonic bonds.

Weak polyelectrolytes can modulate their charge in response to external perturbations, such as changes in the pH, ionic strength (I), or electrostatic interactions with other charged species, a phenomenon known as charge regulation (CR). On the other hand, it is well established that CR is highly coupled with the conformational degrees of freedom. In this paper, the influence of CR in the stretching properties of weak polyelectrolytes is analyzed, and the possibility of CR induced by mechanical stretching is explored. With this aim, we make use of a minimal model, which captures the fundamental aspects present in the stretching of a flexible weak linear polyelectrolyte: internal angle rotation, bond stretching, bond bending, and proton binding, which is the paradigmatic mechanism of CR. Mechanical stretching is studied by performing semi-grand canonical Monte Carlo simulations at different pH and ionic strength conditions.
Effect of set up protocols on the accuracy of alchemical free energy calculation over a set of ACK1 inhibitors.


Hit-to-lead virtual screening frequently relies on a cascade of computational methods that starts with rapid calculations applied to a large number of compounds and ends with more expensive computations restricted to a subset of compounds that passed initial filters. This work focuses on set up protocols for alchemical free energy (AFE) scoring in the context of a Docking – MM/PBSA – AFE cascade.
III.2 PUBLICATION LIST

PUBLISHED ARTICLES

1. \( \text{La}_{1.5}\text{Sr}_{0.5}\text{NiMn}_{0.5}\text{Ru}_{0.5}\text{O}_6 \) double perovskite with enhanced ORR/OER bifunctional catalytic activity.

   B. Wang, P. H. Walton, C. Rovira.

3. Adsorption preference determines segregation direction: a shortcut to more realistic surface models of alloy catalysts.

4. Kinetic Monte Carlo simulations unveil synergic effects at work on bifunctional catalysts.
   H. Prats, S. Posada-Pérez, J. A. Rodríguez, R. Sayós, F. Illas.

5. Outlining the scaling-based and scaling-free optimization of electrocatalysts.
   N. Govindarajan, M. T. M. Koper, E. J. Meijer, F. Calle-Vallejo.


7. What can infrared spectra tell us about the crystallinity of nanosized interstellar silicate dust grains?

8. Structure and properties of nanosilicates with olivine \((\text{Mg}_2\text{SiO}_4)_N\) and pyroxene \((\text{MgSiO}_3)_N\) compositions.
9. Oxidative cleavage of cellobiose by lytic polysaccharide monooxygenase (LPMO)-
inspired copper complexes.
A. C. Neira, P. R. Martínez-Alanis, G. Aullón, M. Flores-Alamo, P. Zerón, A. Company, J.
ACS Omega 4 (2019) 10729-10740.

10. Subsurface carbon – a general feature of noble metals.

11. Enhanced electroreduction of carbon dioxide to methanol using zinc dendrites pulse-
deposited on silver foam.
Q. H. Low, N. W. X. Loo, F. Calle-Vallejo, B. S. Ye.

12. The periodic table – a universal icon: its birth 150 years ago, and its popularization
through literature, art and music.
S. Shaik, E. Cremades, S. Alvarez.

M. López-Martínez, M. López-Ortiz, M. E. Antinori, E. Wientjes, A. Nin-Hill, C. Rovira, R.
Croce, I. Díez-Pérez, P. Gorostiza.

14. [UF6]²: A molecular hexafluorido actinide(IV) complex with compensating spin and orbital
magnetic moments.
K. S. Pedersen, K. R. Meihaus, A. Rogalev, F. Wilhelm, D. Aravena, M. Amoza, E. Ruiz,
J. R. Long, J. Bendix, R. Clerac.

15. A proposal for evading the measurement uncertainty in classical and quantum
computing: application to a resonant tunneling diode and a Mach-Zehnder interferometer.

16. Pharmacology and preclinical validation of a novel anticancer compound targeting
PEPCK-M.
M. Aragó, J. Moreno-Felici, S. Abás, S. Rodríguez-Arévalo, P. Hyrossová, A. Figueras, F.
Viñals, B. Pérez, M. I. Loza, J. Brea, P. Latorre, J. A. Carrodeguas, P. M. García-Rovés,

17. A photoswitchable GABA receptor channel blocker.
G. Maleeva, D. Wutz, K. Rustler, A. Nin-Hill, M. Alfonso-Prieto, E. Petukhova, A.
Bautista-Barrufet, A. Gomila-Juaneda, P. Scholze, F. Peiretti, C. Rovira, B. König, P.
Gorostiza, P. Bregestovski.
   J. Jover.


20. *Conformational effects of [Ni₂(µ-SAr)₂] cores on their electrocatalytic activity.*

21. *Slow-spin relaxation of a low-spin S = 1/2 Fe³⁺ carborane complex.*

22. *Open-shell jellium aromaticity in metal clusters.*
    J. Poater, M. Solà.

23. *Assessing the usefulness of transition metal carbides for hydrogenation reactions.*

24. *Pressure selection for non-reactive and reactive pressure-swing distillation.*

25. *Castor oil biorefinery: conceptual process design, simulation and economic analysis.*

26. *Hydration of cyclohexene to cyclohexanol in a hybrid reactive distillation with a side decantar.*

27. *Integrated reaction-separation processes sequencing and screening at early stages of design.*

29. *Effects of temperature on the shape and symmetry of molecules and solids.*

30. *Ammonia–borane derived BN fragments trapped on bi- and trimetallic titanium(III) systems.*
E. del Horno, J. Jover, M. Mena, A. Pérez-Redondo, C. Yélamos.


32. *IUPAC in Brussels in 1921: a historical photo.*
E. Homburg, D. Fauque, P. J. T. Morris, F. Calascibetta, S. Alvarez.

33. *Computational exploration of NO single-site disproportionation on Fe-MOF-5.*

34. *Approaching multiplet splitting in X-ray photoelectron spectra by density functional theory methods: NO and O2 molecules as examples.*

35. *Carbon monoxide insertion at a heavy p-block element: unprecedented formation of a cationic bismuth carbamyol.*

36. *Revealing the nature of active sites in electrocatalysis.*

37. *α-D-Gal-cyclophellitol cyclosulfamidate is a Michaelis complex analog that stabilizes therapeutic lysosomal α-galactosidase A in Fabry disease.*

38. *Spectral variability in phycocyanin cryptophyte antenna complexes is controlled by changes in the α-polypeptide chains.*
III. SCIENTIFIC ACTIVITY OF IQTCUB MEMBERS


40. *Influence of van der Waals interactions on the solvation energies of adsorbates at Pt-based Eelectrocatalysts.*

41. *Using density functional calculations to elucidate atomic ordering of Pd-Rh nanoparticles at sizes relevant for catalytic applications.*

42. *Computational modeling of transition temperatures in spin-crossover systems.*

43. *Theoretical justification of stable ferromagnetism in ferroelectric BiFeO$_3$ by first-principles.*

44. *Marvellous molecular shapes.*

45. *Experimental and theoretical study of Pb···S and Pb···O sigma-hole interactions in the crystal structures of Pb(II) complexes.*

46. *Designing of antiferromagnetically coupled mono-, di- and tri-bridged copper(II) based catecholase models by varying “auxiliary part” of ligand and anionic co-ligand.*

47. *Effect of the substituents on the nature and strength of lone pair-carbonyl interactions in acyl halides.*

III. SCIENTIFIC ACTIVITY OF IQTCUB MEMBERS

49. *Modeling catalytic reaction mechanisms in glycoside hydrolases.*
    J. Coines, L. Raich, C. Rovira.

50. *Single-ion magnetic anisotropy in a vacant octahedral Co(II) complex.*

51. *Microwave assisted synthesis of heterometallic 3d–4f M₄Ln complexes.*

52. *Dinuclear Co²⁺Yᵐᵢᵣ vs. tetranuclear Co²⁺₂Y₃ᵢᵣ complexes: the effect of increasing molecular size on magnetic anisotropy and relaxation dynamics.*

53. *Computational assessment on the Tolman cone angles for P-ligands.*
    J. Jover, J. Cirera.


55. *Trinuclear gold–carborane cluster as a host structure.*

56. *Electronic structure of the α- (BEDT-TTF)₂I₃ surface by photoelectron spectroscopy.*

57. *A model for a driven Frenkel-Kontorova chain.*
    W. Quapp, J. M. Bofill.

58. *Sliding paths for series of Frenkel-Kontorova models - a contribution to the concept of 1D-superlubricity.*
    W. Quapp, J. M. Bofill
III. SCIENTIFIC ACTIVITY OF IQTCUB MEMBERS

59. *Pt/\text{CeO}_2* and *Pt/\text{CeSnO}_x* catalysts for low-temperature CO oxidation prepared by plasma-arc technique.

60. Oxygen vacancies in oxide nanoclusters: when silica is more reducible than titania.
A. Cuko, S. T. Bromley, M. Calatayud.

61. Ion-pair formation in neutral potassium-neutral pyrimidine collisions: electron transfer experiments.
M. Mendes, B. Pamplona; S. Kumar, F. Ferreira da Silva, A. Aguilar; G. García; M-C Bacchus-Montabonel, P. Limao-Vieira.

62. Conformational itinerary of sucrose during hydrolysis by retaining amylosucrase.
S. Alonso-Gil, J. Coines, I. André, C. Rovira.

63. Toward understanding calmodulin plasticity by molecular dynamics.

64. Lipophilicity in drug design: an overview of lipophilicity descriptors in 3D-QSAR studies.

65. Charge delocalization, oxidation states and silver mobility in the mixed silver-copper oxide *AgCuO*$_2$.

66. On the silicon-silicon bonds σ-coordinated to group 10 transition metals.
G. Aullón.

67. Control over near-ballistic electron transport through formation of parallel pathways in a single-molecule wire.

68. Room temperature methane capture and activation by Ni clusters supported on TiC(001): effects of metal carbide interactions on the cleavage of the C-H bond.

70. Fenton-derived OH radicals enable the MPnS enzyme to convert 2-hydroxyethylphosphonate to methylphosphonate: insights from *ab initio* QM/MM MD simulations.
   B. Wang, Z. Cao, C. Rovira, J. Song, S. Shaik.

71. Calculating the partition coefficients of organic solvents in octanol/water and octanol/air.

72. Understanding the mechanism of direct activation of AMP-kinase: toward a fine allosteric tuning of the kinase activity.

73. Efficient preparation of TiO$_2$ nanoparticles models using interatomic potentials.

74. Electronic properties of realistic anatase TiO$_2$ nanoparticles from G$_0$W$_0$ calculations on a gaussian and plane wave scheme.

75. Interplay between the gentlest ascent dynamics method and conjugate directions to locate transition states.

76. PyFrag 2019 – Automating the exploration and analysis of reaction mechanisms.
   X. Sun, T. M. Soini, J. Poater, T. A. Hamlin, F. M. Bickelhaupt.

77. Prediction of the n-octanol/water partition coefficients in the SAMPL6 blind challenge from MST continuum solvation calculations.
   W. J. Zamora, S. Pinheiro, K. German, C. Ràfols, C. Curutchet, F. J. Luque.

78. Identification of dihydrofuro[3,4-d]pyrimidine derivatives as novel HIV-1 non-nucleoside reverse transcriptase inhibitors with promising antiviral activities and desirable physicochemical properties.
79. Exploiting the tolerant region I of the non-nucleoside reverse transcriptase inhibitor (NNRTI) binding pocket: discovery of potent diarylpyrimidine-typed HIV-1 NNRTIs against wild-type and E138K mutant virus with significantly improved water solubility and favorable safety profiles.

80. Probing through-space polar-pi interactions in 2,6-diarylphenols.

81. “Aggregation-induced emission” of transition metal compounds: design, mechanistic insights, and applications.

82. Understanding H₂ formation on hydroxylated pyroxene nanoclusters: ab initio study of the reaction energetics and kinetics.
B. Kerkeni, M-C.Bacchus-Montabonel, X. Shan, S. T. Bromley.

83. Understanding competition of polyalcohol dehydration reactions in hot water.

84. Surface activity of early transition metal oxycarbides: CO₂ adsorption case study.
C. Kunkel, F. Viñes, F. Illas.

85. Affordable estimation of solvation contributions to the adsorption energies of oxygenates on metal nanoparticles.
F. Calle-Vallejo, R. de Morais, F. Illas, D. Loffreda, P. Sautet.

86. Combining theory and experiment for a multitechnique characterization of activated CO₂ on transition metal carbide (001) surfaces.

87. Pd segregation on the surface of bimetallic PdAu nanoparticles induced by low coverage of adsorbed CO.
88. **Correcting flaws in the assignment of nitrogen chemical environments in n-doped graphene.**

89. **Approaching the quantitative description of enantioselective adsorption by the density functional means.**
   F. Viñes, O. Lamiel-Garcia.

90. **Optical properties and chemical ordering of Ag-Pt nanoalloys: a computational study.**

91. **Grazynes: carbon-based two-dimensional composites with anisotropic properties.**
   S. Kamalinahad, F. Viñes, P. Gamallo.

92. **Development of a structure-based pH-dependent lipophilicity scale of amino acids from continuum solvation calculations.**

93. **Modulating ligand dissociation through methyl isomerism in accessory sites: binding of retinol to cellular carriers.**

94. **Effect of charge regulation and conformational equilibria in the stretching properties of weak polyelectrolytes.**
   P. M. Blanco, S. Madurga, F. Mas, J. L. Garcés.

95. **The role of vibrational anharmonicity in the computational study of thermal spin crossover.**
   J. Wu, C. Sousa, C. de Graaf.

96. **Newton trajectories for the tilted Frenkel-Kontorova model.**
   W. Quapp, J. M. Bofill.

97. **The gas phase oxidation of HCOOH by Cl and NH_2 radicals. Proton coupled electron transfer versus hydrogen atom transfer.**
   J. M. Anglada, R. Crehuet, A. Solé.
98. Understanding the interplay between size, morphology and energy gap in photoactive TiO$_2$ nanoparticles.

99. Fast identification of optimal pure platinum nanoparticle shapes and sizes for efficient oxygen electroreduction.
M. Rück, A. Bandarenka, F. Calle-Vallejo, A. Gagliardi.

100. Structural principles to steer the selectivity of the electrocatalytic reduction of aliphatic ketones on platinum.
C. J. Bondue, F. Calle-Vallejo, M. C. Figueiredo, M. T. M. Koper.

101. Deciphering the enzymatic mechanism of sugar ring contraction in UDP-apiose biosynthesis.

102. Discovery of processive catalysis by an exo-hydrolase with a pocket-shaped active site.

103. Na-doped ruthenium perovskite electrocatalysts with improved oxygen evolution activity and durability in acidic media.

104. Advances and challenges in understanding the electrocatalytic conversion of carbon dioxide to fuels.
Y. Y. Birdja, E. Pérez-Gallent, M. C. Figueiredo, A. J. Göttle, F. Calle-Vallejo, M. T. M. Koper.

105. Mapping of the working route of phosphatase activity of copper based models with special emphasis on the role of oxo-anions by combined experimental and theoretical studies.
106. *Supramolecular tripodal Au(I) assemblies in water. Interactions with pyrene fluorescent probe.*

107. *Applying discriminant and cluster analyses to separate allergenic from non-allergenic proteins.*
   L. Naneva, M. Nedyalkova, S. Madurga, F. Mas, V. Simeonov.


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

110. *Glucose transport via the pseudomonads porin OprB. Implications for the design of trojan-horse antinfectives.*

111. *Effect of electron correlation in the decomposition of core level binding energy shifts into initial and final state contributions.*

112. *Understanding the differences between iron and palladium in cross-coupling.*

113. *Double-well potential energy in the interaction between h-BN and Ni(111).*

114. *Conformational analysis of enantiomerization coupled to internal rotation in triptycyl-n-helicenes.*

115. *Revising the common understanding of metamagnetism in the molecule-based bisdithiazolyl BDTMe compound.*
116. CeO$_2$(111) electronic reducibility tuned by ultra-small supported bimetallic Pt-Cu clusters.

117. *Implicit solvent effect in the determination of Bronsted-Evans-Polanyi relationships for heterogeneously catalyzed reactions.*

118. *Rotational energy relaxation quantum dynamics of a diatomic molecule in a superfluid helium nanodroplet and study of the hydrogen isotopes case.*
M. Blancafort-Jorquera, A. Vilà, M. González.


120. *Thickness biased capture of CO$_2$ on carbide MXenes.*
Á. Morales-García, M. Mayans-Llorach, F. Viñes, F. Illas.

121. *Quantum-classical approach to the reaction dynamics in a superfluid helium nanodroplet. The Ne$_2$ dimer and Ne-Ne adduct formation reaction Ne + Ne-doped nanodroplet.*
M. Blancafort-Jorquera, A. Vilà, M. González.

122. *Electron self-organization in NbSe$_3$ revealed by polarization-dependent nano-ARPES.*

123. *Fermi surface properties of the bifunctional organic metal κ-(BETS)$_2$Mn[N(CN)$_2$]$_3$ near the metal–insulator transition.*

124. *Selective nanomechanics of aromatic versus aliphatic thiolates on gold surfaces.*

125. *Nonadiabatic quantum dynamics without potential energy surfaces.*
126. *Effect of set up protocols on the accuracy of alchemical free energy calculation over a set of ACK1 inhibitors.*

127. *Interaction of human hemoglobin and semi-hemoglobins with the Staphylococcus aureus hemophore IsdB: a kinetic and mechanistic insight.*

128. *Silver atom, trimer and tetramer species supported on a ceria nanoparticle: a density functional study.*

129. *Study of active surface centers of Pt/CeO₂ catalysts prepared using radio-frequency plasma sputtering technique.*

130. *Differential many-body effects for initial and core-ion states: impact on XPS spectra.*

131. *Electronic energy transfer in biomacromolecules.*
L. Cupellini, M. Corbella, B. Mennucci, C. Curutchet.
BOOK CHAPTERS AND PROCEEDINGS

1. *150 Anys de Taules Periòdiques a la UB.*

2. *100 Curiositats sobre la Taula Periòdica i els elements químics.*
S. Alvarez, author of some chapters.

3. *How to design models for ceria nanoparticles: challenges and strategies for describing nanostructured reducible oxides.*
A. Bruix, K.M. Neyman.

4. *Fractal Dimension (FD).*
P. M. Blanco, S. Madurga, A. Isvoran, L. Pitulice, F. Mas.

5. *Fractal Kinetics (FK).*

6. *Macromolecular Crowding (MC).*

7. *Simulation paths of anticancer drugs on a graphene oxide surface.*
III. SCIENTIFIC ACTIVITY OF IQTCUB MEMBERS

III.3 OTHER ACTIVITIES

PHD THESSES 2019

1. Toward refined theoretical models for the description of lipophilicity in biomolecules.
   William J. Zamora
   PhD program: Biotechnology.
   Faculty of Pharmacy and Food Sciences, University of Barcelona.
   February 2019

2. Rationalization of the mechanism of bistability in dithiazolyl-based molecular magnets.
   Tommaso Francese
   PhD program: Theoretical Chemistry and Computational Modelling.
   Faculty of Chemistry, University of Barcelona.
   Supervisor/s: J. J. Novoa Vide, Ria Broer.
   March 2019.

3. Monte Carlo based methods applied to heterogeneous catalysis and gas separation.
   Héctor Prats García
   PhD program: Theoretical Chemistry and Computational Modelling.
   Faculty of Chemistry, University of Barcelona.
   Supervisor/s: Ramón Sayós, Francesc Illas.
   March 2019.

4. Desarrollos metodológicos en la exploración de la especie bioactiva en fármacos: Búsqueda de agentes antimaláricos.
   Antonio Viayna Gaza
   PhD program: Biotechnology.
   Faculty of Pharmacy and Food Sciences, University of Barcelona.
   Supervisor/s: F. J. Luque.
   June 2019.

5. On the usage of lipophilic descriptors for molecular similarity evaluation.
   Javier Vázquez Lozano
   PhD program: Biotechnology.
   Faculty of Pharmacy and Food Sciences, University of Barcelona.
   Supervisor/s: F. J. Luque, Enric Herrero.
   September 2019.
6. *Models and computational methods applied to industrial gas separation processes and enhanced oil recovery.*

**Gerard Alonso Benito**
PhD program: Theoretical Chemistry and Computational Modelling.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: Ramón Sayós, Pablo Gamallo.
November 2019.

7. *Anisotropía en imanes unimoleculares y qubits con complejos metálicos con espin S = 1/2.*

**Martín Amoza Dávila**
PhD program: Molecular Inorganic Chemistry.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: E. Ruiz.
November 2019.

8. *Theoretical reaction and relaxation dynamics in superfluid helium nanodroplets.*

**Miquel Blancafort Jorquera**
PhD program: Theoretical Chemistry and Computational Modelling.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: Miguel González.
November 2019.


**Cristina Balcells Nadal**
PhD program: Molecular Biotechnology.
Faculty of Chemistry, University of Barcelona.
Supervisor/s: Marta Cascante, Francesc Mas.
December 2019.
III. SCIENTIFIC ACTIVITY OF IQTCUB MEMBERS

MASTER THESES 2019

1. *Simulation and experimental struvite crystallization with real waste water.*
   **Víctor Alcaraz Esteban**  
   MSc program: Chemical Engineering.  
   Faculty of Chemistry, University of Barcelona.  
   Supervisor/s: Alexandra Plesu Popescu, Joan Llorens Llacuna.  
   February 2019.

2. *CFD Analysis of mass transfer, shear stress and hydrodynamics in a lab apparatus to test forward osmosis membranes.*
   **Álex Terradillos Guillén**  
   MSc program: Chemical Engineering.  
   Faculty of Chemistry, University of Barcelona.  
   Supervisor/s: Alexandra Plesu Popescu, Joan Llorens Llacuna.  
   April 2019.

3. *CFD study of NOx emissions decreases by flame additives.*
   **Hector Joel López Molina**  
   MSc program: Chemical Engineering.  
   Faculty of Chemistry, University of Barcelona.  
   Supervisor/s: Alexandra Plesu Popescu, Jordi Bonet i Ruiz.  
   April 2019.

4. *Optimization of ethanol and ethyl acetate separation by pressure swing distillation.*
   **Víctor Manso Álvarez**  
   MSc program: Chemical Engineering.  
   Faculty of Chemistry, University of Barcelona.  
   Supervisor/s: Alexandra Plesu Popescu, David Curcó Cantarell.  
   April 2019.

5. *Insights on Mo activity in deoxygenation reactions.*
   **Biel Martinez Diaz**  
   MSc program: Theoretical Chemistry and Computational Modelling.  
   Faculty of Chemistry, University of Barcelona.  
   Supervisor/s: Francesc Viñes.  
   June 2019.

   **José Luis Pellín Moreno**  
   MSc program: Chemical Engineering.  
   Faculty of Chemistry, University of Barcelona.  
   Supervisor/s: Alexandra Plesu Popescu, Manuel Vicente Buil.  
   June 2019.
III. SCIENTIFIC ACTIVITY OF IQTCUB MEMBERS

7. **CFD Modelling with MFIX® of liquid-solid fluidized beds of polydisperse struvite crystals.**
   **Ricardo Moya Chamizo**
   MSc program: Chemical Engineering.
   Faculty of Chemistry, University of Barcelona.
   Supervisor/s: Alexandra Plesu Popescu, Ricard Torres Castillo.
   June 2019.

8. **Water cycle management and indicators: a review.**
   **Aitor Barroso Roig**
   MSc program: Environmental Engineering.
   Faculty of Chemistry, University of Barcelona.
   Supervisor/s: Alexandra Plesu Popescu, Jordi Bonet i Ruiz.
   June 2019.

9. **Surrogate model for chemical absorbents mixtures for CO₂ capture.**
   **Enric Sefla Martínez**
   MSc program: Environmental Engineering.
   Faculty of Chemistry, University of Barcelona.
   Supervisor/s: Alexandra Plesu Popescu, Jordi Bonet i Ruiz.
   June 2019.

10. **ANSYS Fluent simulation of a conventional chimney.**
    **Roger Pitarch Greis**
    MSc program: Environmental Engineering.
    Faculty of Chemistry, University of Barcelona.
    Supervisor/s: Alexandra Plesu Popescu, Ricard Torres Castillo.
    June 2019.

11. **Comprehensive study of carbon dioxide hydrogenation over Ni (111) surface: reverse Water-Gas Shift reaction vs. Sabatier reaction.**
    **Pablo Lozano-Reis**
    MSc program: Theoretical Chemistry and Computational Modelling.
    Faculty of Chemistry, University of Barcelona.
    Supervisor/s: Pablo Gamallo, Ramón Sayós.
    July 2019.

12. **Unravelling calmodulin conformational ensemble from combined molecular dynamics and FRET simulations.**
    **Daniel Gonzalo Palao**
    MSc program: Environmental Engineering.
    Faculty of Pharmacy and Food Sciences, University of Barcelona.
    Supervisor/s: Carles E. Cuturchet.
    July 2019.

13. **Study of the transglycosylation complex of β-galactosidase using molecular dynamics.**
    **Iker Zapirain Gysling**
    MSc program: Theoretical Chemistry and Computational Modelling.
    Faculty of Chemistry, University of Barcelona.
    Supervisor/s: Carme Rovira.
    July 2019.
14. *Theoretical insight into the active site dynamics of fucosyltransferases.*

**Beatriz Piniello Castillo**
MSc program: Atomistic and Multiscale Computational Modelling in Physics, Chemistry and Biochemistry.  
Faculty of Chemistry, University of Barcelona.  
Supervisor/s: Carme Rovira.  
July 2019.

15. *Disociación de CO$_2$ catalizada por MXenes.*

**Raul Morales Salvador**
MSc program: Atomistic and Multiscale Computational Modelling in Physics, Chemistry and Biochemistry.  
Faculty of Chemistry, University of Barcelona.  
Supervisor/s: Ángel Morales-García, Francesc Viñes.  
July 2019.

16. *First-principles evaluation of the initial oxidation of transition metal surfaces.*

**Anabel Jurado Mañas**
MSc program: Chemistry of Advanced Materials.  
Faculty of Chemistry, University of Barcelona.  
Supervisor/s: Francesc Viñes.  
July 2019.

17. *Relacions estructura/propietats magnètiques a la unitat [Dy$_2$(RCOO)$_4$].*

**Alba Palacios Requena**
MSc program: Theoretical Chemistry and Computational Modelling.  
Faculty of Chemistry, University of Barcelona.  
Supervisor/s: Jordi Cirera.  
July 2019.

18. *Desenvolupament d’un camp de forces per primers principis per a gàbies metal·lo-òrgàniques de [Fe$_4$].*

**Laia Navarro Maestro**
MSc program: Atomistic and Multiscale Computational Modelling in Physics, Chemistry and Biochemistry.  
Faculty of Chemistry, University of Barcelona.  
Supervisor/s: Jordi Cirera.  
July 2019.

19. *Quantum chemical examination of the influence of substituents on the spin crossover temperature of manganocenes.*

**Florian Matz**
Faculty of Chemistry, University of Barcelona & Institut für Physikalische Chemie und Elektrochemie (Hannover, Germany).  
Supervisor/s: Jordi Cirera.  
July 2019.
20. Setting up a methodology to decipher cryptic pockets.  
Pol Costas Viñas  
MSc program: Theoretical Chemistry and Computational Modelling.  
Faculty of Sciences, Autonomous University of Madrid.  
Supervisor/s: Jaime Rubio Martínez.  
July 2019.

Kassiani Motaki  
MSc program: Theoretical Chemistry and Computational Modelling.  
Faculty of Chemistry, University of Barcelona.  
Supervisor/s: Jaime Rubio Martínez.  
July 2019.

22. Quest for compounds that selectively activate the pro-apoptotic Bax protein.  
Natàlia de Moya Valenzuela  
MSc program: Theoretical Chemistry and Computational Modelling.  
Faculty of Chemistry, University of Barcelona.  
Supervisor/s: Jaime Rubio Martínez.  
July 2019.

23. Chemical ordering in Ag-Pt nanoalloys: structures and spectra.  
Sofia Olobardi  
MSc program: Chemistry.  
Dipartimento di Scienze Chimiche e Farmaceutiche, Università di Trieste, Italy.  
Supervisor/s: Mauro Stener, Konstantin Neyman.  
July 2019.

24. New computational strategies to obtain kinetic data of enzymatic processes in crowded media.  
Raquel Agraso Riobó  
MSc program: Atomistic and Multiscale Computational Modelling in Physics, Chemistry and Biochemistry.  
Faculty of Chemistry, University of Barcelona.  
July 2019.

25. How to accurately model the IR spectra of cosmic nanosilicate dust grains.  
Joan Mariñoso Guiu  
MSc program: Theoretical Chemistry and Computational Modelling.  
Faculty of Chemistry, University of Barcelona.  
Supervisor/s: Stefan T. Bromley.  
July 2019.

26. Modelling lacto-n-biosidase from Bifidobacterium bifidum by means of molecular dynamics.  
Irene Cuxart Sánchez  
MSc program: Bioengineering.  
Institut Químic de Sarrià, Ramon Llull's University.  
Supervisor/s: Carme Rovira.  
September 2019.
III. SCIENTIFIC ACTIVITY OF IQTCUB MEMBERS

SCIENTIFIC CONFERENCES AND MEETINGS 2019

Scientific Advisory Board Meeting of the MPSD
Hamburg (Germany) 9 January 2019

Trajectory Approaches for Nonequilibrium Quantum Dynamics in Light-Matter Systems
(post)

10th Symposium on Computing π-Conjugated Compounds
Valencia (Spain) 31 January – 2 February 2019

Understanding spectral variability in cryptophyte antenna complexes from multiscale simulations (oral communication)
C. Curutchet

Chemistry Today for Tomorrow (Science and Education for Smart Growth)
Sofia (Bulgaria) 1 February 2019

New descriptions for proteins: separation of allergenic from non-allergenic proteins (oral communication)
S. Madurga, M. Nedyalkova, F. Mas, V. Simeonov

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

Theoretical modeling of the transition temperature in spin-crossover molecules (oral communication)
J. Cirera

Spin transition in dithiazolyl based switchable materials (oral communication)
J. Ribas

Influence of charge regulation on conformational, ionization and stretching properties of polyelectrolytes (oral communication)
F. Mas, P. M. Blanco, S. Madurga, J. L. Garcés

Polymer-Borate hybrids films - Theoretical and experimental determination of the structure (poster)
H. Hristov, M. Nedyalkova, S. Madurga
Borosilicate hybrid materials and nanocomposites: synthetic, structural and statistical approach (poster)
H. Hristov, M. Nedyalkova, S. Madurga, V. Simeonov

Predicting partition coefficients by first principles calculations of organic solvents with implicit solvent model (poster)
M. Nedyalkova, S. Madurga, M. Tobiszewski, V. Simeonov

Presentació de l’Any Internacional de la Taula Periòdica
Barcelona (Spain) 5 February 2019

Presentació de peces musicals a l’Institut del Teatre (invited talk)
S. Alvarez

GrapheneforUS International Conference
New York (USA) 14-15 February 2019

CO₂ Chemical Trapping on Two-Dimensional MXenes (oral communication)
Á. Morales-García, F. Viñes, R. Morales-Salvador, F. Illas

Les mil cares de la taula periòdica (cicle de conferències de la Biblioteca de la Vila de Gràcia)
Barcelona (Spain) 18 February 2019

La taula periòdica com a referent cultural (invited talk)
S. Alvarez

APS Spring Meeting
Boston (USA) 4-8 March 2019

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

Molecular Dynamics Today (MD2d)
Bologna (Italy) 14-15 March 2019

Toward a comprehensive understanding of the mechanisms of biological activity with molecular simulations (oral communication)
F. J. Luque
III. SCIENTIFIC ACTIVITY OF IQTCUB MEMBERS

6th Computationally Driven Drug Discovery (CDDD) Meeting
Rome (Italy) 28-29 March 2019

On the Usage of Novel Hydrophobic Molecular Fields for CADD (oral communication)
A. DePlano, O. Rey, J. Vázquez, A. Herrero, E. Gibert, E. Herrero, F. J. Luque

ACS National Meetings
Orlando (USA) 31 March – 2 April 2019

Morphology Dependence of Stability and Properties of Stoichiometric TiO$_2$ Nanoparticles
(oral communication)
Á. Morales-García, A. Macià, S. T. Bromley, F. Illas

CECAM School on Hybrid Quantum Mechanics / Molecular Mechanics (QM/MM)
Approaches to Biochemistry and beyond
Lausanne (Switzerland) 8-12 April 2019

C. Rovira (organization)

CECAM School on Kinetics and Dynamics of Chemical Reactions
Zaragoza (Spain) 8-12 April 2019

P. Gamallo (organization)

Kinetic Monte Carlo Simulations (seminar)
P. Gamallo

Molecular Dynamics (seminar)
X. Giménez

Calculating kinetic coefficients of chemical reactions using quantum dynamics (seminar)
F. Huarte-Larrañaga

Wave-packet quantum Dynamics: overview and Applications to chemical reactions (seminar)
P. Gamallo
III. SCIENTIFIC ACTIVITY OF IQTCUB MEMBERS

International Astronomical Union: S350 Laboratory Astrophysics
Cambridge (United Kingdom) 14 April 2019

Using Atomistically Detailed Simulations to Understand the Formation, Structure and Composition of Astrophysical Silicate Dust Grains (oral communication)
S. T. Bromley

Centre in Green Chemistry and Catalysis (CGCC) 10th Annual Symposium
Montreal (Canada) 11 May 2019

Insights in Mo₂C activity in deoxygenation reactions (poster)
B. Martínez, F. Viñes, P. McBreen, F. Illas

25th Topical Meeting of the International Society of Electrochemistry
Toledo (Spain) 12-15 May 2019

Why breaking scaling relations does not necessarily lead to better electrocatalysts (oral communication)
Federico Calle-Vallejo

FOTOFUEL Workshop on Solar Fuels
Madrid (Spain) 13-14 Maig 2019

Unbiased Analysis of the Interplay between Size, Morphology and Energy Gap in Realistic TiO₂ Nanoparticles (invited talk)
Á. Morales-García

13th Carbohydrate Bioengineering Meeting (CBM13)
Toulouse (France) 19 May 2019

Early stages of glycogen biosynthesis: mechanism of action of glycogenin (oral communication)
C. Rovira

Oxazoline or oxazolinium ion? The reaction mechanism of GH18 chitinases (oral communication)
J. Coines, M. Alfonso-Prieto, X. Biarnés, A. Planas, C. Rovira
III. SCIENTIFIC ACTIVITY OF IQTCUB MEMBERS

World Chemistry Forum 2019
Barcelona (Spain) 22-24 May 2019

Novel catalysts for methane activation at room temperature (keynote talk)
F. Illas

Effects of oxide supports on reactivity of metal particles in catalysis and energy technologies (invited talk)
K. M. Neyman

XXXVII Reunión Bienal de la Real Sociedad Española de Química
Donostia (Spain) 26-30 May 2019

Multiscale modeling of light harvesting in cryptophyte photosynthesis (oral communication)
C. Curutchet

Games with the Periodic Table to increase public awareness of science (oral communication)
J. Poater, S. Simon, M. Miquel Solà, M. Duran

New Trends in Statistical Physics: 50 years of the Sitges Conference
Sitges (Spain) 27-31 May 2019

Weak Polyelectrolyte Modelling: Coupling Charge Regulation and Conformational Equilibria vis LEIP Methodology (poster)
J. L. Garcés, P. M. Blanco, S. Madurga, F. Mas

A New Model for Macromolecular Diffusion in Crowded Media: the Chain Entanglement Soft Potential (poster)
P. M. Blanco, S. Madurga, J. L. Garcés, F. Mas

MasterQuímica XV
Barcelona (Spain) 28-30 May 2019

Noves estartègies computacionals per obtenir dades cinètiques dels processos enzimàtics en medi aglomerat (poster)
R. Agraso, P. M. Blanco, S. Madurga, F. Mas
Theoretical Chemistry and Computational Modelling: 20 years promoting Excellence in Science (20TCCM)
Donostia (Spain) 30 May – 1 June 2019

Magnetic and Conductive properties in multifunctional bisdithiazolyl-based materials (oral communication)
C. Roncero

Bifunctional catalysts at work: unravelling synergic effects by kinetic Monte Carlo simulations (poster)
R. Sayós, H. Prats, S. Posada-Pérez, J. A. Rodríguez, F. Illas

X Simposium IQTC-UB
Barcelona (Spain) 31 Maig 2019

Jordi Cirera (organization)

A Computational View on Astronomical Silicate Nanoclusters (invited talk)
A. Macià

Mechanistic insights into substrate-assisted glycoside hydrolases (invited talk)
Joan Coines

Rotational relaxation in superfluid helium nanodroplets (poster)
M. Blancafort, A. Vilà, M. González

Vibrational relaxation in superfluid helium nanodroplets (poster)
M. Blancafort, A. Vilà, M. González

Unravelling Calmodulin conformational ensemble from combined Molecular Dynamics and FRET simulations (poster)
D. Gonzalo, C. Curutchet

Correcting Flaws in the Assignment of Nitrogen Chemical Environments in N-Doped Graphene (poster)

Insights on Mo₂C Activity in Deoxygenation Reactions (poster)
B. Martínez, F. Viñes, P. McBreen, F. Illas

Carbon Dioxide Hydrogenation over Nickel Catalysts: DFT and Kinetic Monte Carlo (poster)
P. Lozano, H. Prats, P. Gamallo, F. Illas, R. Sayós

Accuracy of the Topological Approach for Nanoalloys: Case Study of PtCu Nanoparticles (poster)
L. Vega, F. Viñes, K. M. Neyman
How to accurately model IR spectra of silicate granites (poster)
J. Mariñoso, A. Macià, S. T. Bromley

Weak Polyelectrolyte Modelling: Coupling Charge Regulation and Conformational Equilibria vis LEIP Methodology (poster)
J. L. Garcés, P. M. Blanco, S. Madurga, F. Mas

A New Model for Macromolecular Diffusion in Crowded Media: the Chain Entanglement Soft Potential (poster)
P. M. Blanco, S. Madurga, J. L. Garcés, F. Mas

Analysis of the supramolecular structure of helicobacter pyloriurease extracellular at different pHs by molecular dynamics simulation (poster)
H. L. Barazorda-Ccahuana, B. Gómez, F. Mas, S. Madurga

New computational strategies to obtain kinetic data of enzymatic processes in crowded media (poster)
R. Agraso, P. M. Blanco, S. Madurga, F. Mas

Prediction of partition coefficients by ab initio calculations (poster)
L. Saranjian, M. Nedyalkova, V. Simeonov, F. Mas, S. Madurga

Theoretical insight into the active site Dynamics of O-fucosyltransferase 1 (poster)
Beatriz Piniello, C. Rovira

Selective hydrogenation from alkynes into alkenes on transition metal carbide surfaces: C_H activation (poster)
Carlos Andrés Jimenez-Orozco, Elizabeth Florez, Jose Rodriguez

Alzheimer’s disease: What can lipophilicity teach us? (poster)
William J. Zamora, J. M. Campanera, K. P. Kepp, F. J. Luque

Framework electron count and structural trends in [Li2X2] rings (poster)
Juan Diego Velasquez, J. Echeverria, S. Alvarez

An introductory workshop in biomedical glycoscience
Donostia (Spain) 3 June 2019

Modeling catalytic mechanisms in carbohydrate-active enzymes (invited talk)
C. Rovira
III. SCIENTIFIC ACTIVITY OF IQTCUB MEMBERS

Delegació del CSIC
Barcelona (Spain) 3 June 2019

La taula periódica com a icona cultural (invited talk)
S. Alvarez

International Meeting on Nanoalloys 2019 (IMN 2019)
Genoa (Italy) 4-7 June 2019

Accuracy of the Topological Approach for nanoalloys: Case study of PtCu nanoparticles (poster)
L. Vega, F. Viñes, K. M. Neyman

Atomic ordering in large bimetallic particles from DFT+Topological calculations (oral communication)
K. M. Neyman

Exploring Complex Free Energy Landscapes: Structure/Function Formation, Multiscales, and Long-timescales
Mainz (Germany) 5 June 2019

How does nature make glycosidic bonds. Insight from enhanced-sampling QM/MM simulations (invited talk)
C. Rovira

Nordic Polymer Days 2019
Trondheim (Norway) 5-7 June 2019

Exploring mechanically-induced charge regulation in weak polyelectrolytes by computer modelling (oral communication)
P. M. Blanco, J. L. Garcés, F. Mas, S. Madurga

XIIth International School on Organometallic Chemistry “Marcial Moreno Mañas”
Castelló de la Plana (Spain) 12-14 June 2019

DFT studies on copper-catalyzed hydroboration/C–C bond formation reactions (oral communication)
J. Jover, E. Ruiz
3rd International Congress of Chemical Engineering (ANQUE-ICCE)
Santander (Spain) 17-18 June 2019

P. Gamallo (chairman scientific session)

Molecular modelling applied to post-combustion CO₂ capture and separation (oral communication)

1st Congreso Iberoamericano de Ingeniería Química (CIBIQ)
Santander (Spain) 19-21 June 2019

New materials from computational simulations (oral communication)
S. Kamalinahad, F. Viñes, P. Gamallo

Modelling of phosphonium-based ILs for gas separation from the combination of the soft-SAFT equation of state and COSMO-RS techniques (oral communication)
G. Alonso, P. Gamallo, R. Sayós, F. Llovell

Bioheterocycles 2019. XVIII International Conference on Heterocycles in Biorganic Chemistry
Ghant (Belgium) 20 June 2019

Biradical formation by deprotonation in conjugate 2-amino/imino thiazole derivatives (poster)

Milestones in Molecular Simulations
London (United Kingdom) 21 June 2019

How carbohydrate-active enzymes work. Insight from enhanced-sampling QM/MM simulations (invited talk)
C. Rovira

5th EUCheM Inorganic Chemistry Conference (EICC-5)
Moscow (Russia) 24-28 June 2019

Computational Modeling of Transition Temperatures in Spin-Crossover Systems (oral communication)
J. Cirera
Computational study of NO single-site disproportionation on Fe\(^{II}\)(MOF-5) (oral communication)
J. Jover, C. K. Brozek, M. Dincă, N. López

9è Curs d’Introducció a la Química Computacional (IQTCUB)
Barcelona (Spain) 25-28 June 2019

G. Aullón (coordinator)

Universidade Nova de Lisboa
Caparica (Portugal) 26 June 2019

The Periodic Table as a Cultural Icon (invited talk)
S. Alvarez

26th Thermodynamics Conference
Punta Umbria (Spain) 26-28 June 2019

Assessing salt-surfactant synergistic effects on interfacial tension from molecular dynamics simulations (oral communication)
G. Alonso, P. Gamallo, A. Mejía, R. Sayós

Interfacial properties of the water + hexane mixture along three-phase line (oral communication)
G. Alonso, M. Cartes, A. Mejia, E. A. Müller

Universidade do Minho
Braga (Portugal) 28 June 2019

Photographers of Chemistry: Art and Documentation (invited talk)
S. Alvarez

20th European Carbohydrate Symposium (EUROCARB)
Leiden (Netherlands) 30 June – 4 July 2019

How carbohydrate-active enzymes work. Insight from computer simulation (plenary conference)
C. Rovira
Oxazoline Or Oxazolinium Ion? The Protonation State and Conformation of the Reaction Intermediate of Chitinase Enzymes (oral communication)
J. Coines, M. Alfonso-Prieto, X. Biarnés, A. Planas, C. Rovira

Catalytic mechanism of β - galactosidases (poster)
A. Nin-Hill, L. Raich, C. Rovira

The Sweet Gateway of Pseudomonads: Sugar Transport Across the OprB Porin (poster)
J. Coines, S. Acosta-Gutiérrez, I. Bodrenko, C. Rovira, M. Ceccarelli

Unveiling the molecular mechanism of a novel oligoxylanase (oral communication and poster)

MQM 2019 9th Molecular Quantum Mechanics Conference
Heidelberg (Germany) 5 July 2019

The gentlest ascent dynamics method with conjugate directions: a new and efficient algorithm to locate transition states (poster)

Quantum equilibration in a model system porphine (poster)
J. M. Bofill, G. Albareda, I. de P. R. Moreira

Valence tautomerism in organic and organometallic compounds generates unexpected biradical species: a valence bond interpretation (poster)
I. de P. R. Moreira, J. M. Bofill, R. Valero, G. Albareda

The Frenkel-Kontorova Chain (poster)
W. Quapp, J. M. Bofill

19th Meeting of the Spanish Society of Medicinal Chemistry
Vitoria (Spain) 8-11 July 2019

On the bioactive species of azocine-based AChE inhibitors: Interplay between activity and tautomerism (oral communication)
A. Viayna, S. Antermite, C. Altomare, F. J. Luque

XXXVII Reunión bienal Real Sociedad Española de Física
Zaragoza (Spain) 15-19 July 2019

Quantum dynamics of H₂ in SWCNTs: Eigenstates, diffusion and surface coupling (oral communication)
F. Huarte-Larrañaaga
CECAM Workshop on Recent developments in quantum dynamics
Lyon (France) 17 July 2019

Approaches to nonadiabatic quantum dynamics without potential-energy surfaces (invited talk)
G. Albareda

35ª Reunió Anual de la XRQTC
Barcelona (Spain) 18 July 2019

Francesc Illas, Silvia Chellini (co-organization)

Towards a comprehensive understanding of Pt-based electrocatalysts (invited talk)
Federico Calle-Vallejo

N-Benzyl 4,4-disubstituted piperidines as a potent class of influenza H1N1 virus inhibitors showing a novel mechanism of hemagglutinin fusion peptide interaction (invited talk)
Tiziana Ginex

Vibrational relaxation of diatomic molecules in superfluid helium nanodroplets. Influence of the interaction potential, vibrational energy separation and nanodroplet size (poster)
M. Blancafort, A. Vilà, M. González

A quantum dynamics approach to the rotational relaxation of diatomic molecules inside superfluid helium nanodroplets. Application to some isotope variants of H₂ (poster)
M. Blancafort, A. Vilà, M. González

Unravelling Calmodulin conformational ensemble from combined Molecular Dynamics and FRET simulations (poster)
D. Gonzalo, C. Curutchet

Analysis of the supramolecular structure of helicobacter pyloriurease extracellular at different pHs by molecular dynamics simulation (poster)
H. L. Barazorda-Ccahuana, B. Gómez, F. Mas, S. Madurga

New computational strategies to obtain kinetic data of enzymatic processes in crowded media (poster)
R. Agraso, P. M. Blanco, S. J.L. Garcés, Madurga, F. Mas

Quantum Equilibration in a Model System Porphine (poster)
J. M. Bofill, G. Albareda, I. de P. R. Moreira, R. Valero

Carbon dioxide hydrogenation over the Ni (111) surface: reverse Water-Gas Shift reaction vs Sabatier reaction (poster)
P. Lozano, H. Prats, P. Gamallo, F. Illas, R. Sayós
The 18th International Symposium on Novel Aromatic Compounds (ISNA-18)
Sapporo (Japan) 21 July 2019

Hückel’s rule categorizes aromatic closo-boron hydride clústers (oral communication)
J. Poater

Horizon 2020 Project “Materials Networking” Advanced Materials Workshop
Varna (Bulgaria) 21-25 July 2019

Stability or Photoactivity? Properties of Realistic TiO$_2$ Nanoparticles (oral communication)
Á. Morales-García, A. Macià, S. T. Bromley, F. Illas

Two Dimensional Transition Metal Carbides/Nitrides (MXenes) as Potential Catalysts for CO$_2$ Conversion to CO (oral communication)
R. Morales-Salvador, D. Gouveia, Á. Morales-García, F. Viñes, José R. B. Gomes, F. Illas

Correcting Flaws in the Assignment of Nitrogen Chemical Environments in N-doped Graphene (oral communication)
M. Figueras, I. J. Villar-García, F. Viñes, C. Sousa, V. de la Peña O’Shea, F. Illas

First Principles Evaluation of the Initial Oxidation of Transition Metal Surfaces (oral communication)
A. Jurado-Mañas, F. Viñes

Multiscale modeling of spin-crossover phenomena in molecular materials (oral communication)
J. Cirera

XXVI Encontro Nacional de SPQ
Porto (Portugal) 24-26 July 2019

A computational study on the water splitting reaction by MXenes (oral communication)
D. Gouveia, Á. Morales-García, F. Viñes, F. Illas, J. R. B. Gomes

XXVIII International Materials Research Congress
Cancun (Mexico) 18-23 August 2019

K. M. Neyman (co-organization, chairman scientific session)

Improving accuracy of the topological approach for nanoalloys: Case study of PtCu nanoparticles (poster)
L. Vega, F. Viñes, K. M. Neyman
III. SCIENTIFIC ACTIVITY OF IQTCUB MEMBERS

Accuracy of the topological approach for nanoalloys: Case study of PtCu nanoparticles (poster)
L. Vega, F. Viñes, K. M. Neyman

Metal/metal-oxide interface effects in catalytic nanomaterials: Theory versus experiment (invited talk)
K. M. Neyman

Atomic ordering in large bimetallic particles from DFT+Topological calculations (invited talk)
K. M. Neyman

MCARE 2019
Jeju Island (South Korea) 19-23 August 2019

Designing water splitting catalysts using heuristic rules: advantages, dangers and alternatives (invited talk)
Federico Calle-Vallejo

258th American Chemical Society National Meeting and Exposition
San Diego (USA) 25-29 August 2019

Computational modelling of ceria-based nanocomposite materials for catalysis (invited talk)
K. M. Neyman

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

Light & Life - 2019 ESP-IUPB World Congress
(17th International Congress on Photobiology & 18th Congress of the European Society for Photobiology)
Barcelona (Spain) 25-30 August 2019

Multiscale modeling of light harvesting in cryptophyte photosynthesis (oral communication)
C. Curutchet
III. SCIENTIFIC ACTIVITY OF IQTCUB MEMBERS

CECAM/Psi-K School on Density-functional theory and beyond – high-throughput screening and big-data analytics, towards exascale computational materials science
Barcelona (Spain) 26 August – 5 September 2019

E. Ruiz (organization)

Hands-on-DFT 2019
Barcelona (Spain) 26 August – 6 September 2019

Unraveling Morphological and Topological Key Aspects of Pd Nanoparticles (poster)
L. Vega, F. Viñes, K. M. Neyman

Subsurface Carbon: A General Feature of Noble Metals (poster)
O. Piqué, I. Z. Koleva, F. Viñes, H. A. Aleksandrov, G. N. Vayssilov, F. Illas

Morphology Dependence of Stability and Properties of Stoichiometric TiO₂ Nanoparticles (poster)
Á. Morales-García, A. Macià, S. T. Bromley, F. Illas

CO₂ methanation reaction on the Ni (111) surface: first-principles (poster)
P. Lozano, H. Prats, P. Gamallo, F. Illas, R. Sayós

12th European Conference on Computational and Theoretical Chemistry (EUCO-CTC)
Perugia (Italy) 1-5 September 2019

First-principles-based kinetic Monte Carlo simulations in heterogeneous catalysis: Application to water-gas shift reaction with several catalysts (keynote talk)
R. Sayós, H. Prats, S. Posada-Pérez, J. A. Rodríguez, F. Illas

1st International Conference on Noncovalent Interactions (ICNI2019)
Lisbon (Portugal) 2-6 September 2019

Carbonyl-carbonyl interactions in transition metal complexes (invited talk)
J. Echeverría
Computation and Understanding in Quantum Molecular Science  
Toulouse (France), 3-6 September 2019

*Continuity and Discontinuity in the Periodic Table (invited talk)*  
S. Alvarez

8th IAPC Meeting  
Split (Croatia) 9-11 September 2019

*The influence of the background salt in the n-octanol/water distribution coefficient of ionizable drugs (poster)*  
C. Ràfols, M. Rosés, W. J. Zamora, F. J. Luque

Faraday Discussion: Quantum effects in complex systems  
Coventry (United Kingdom) 11-13 September 2019

*Kinetic Quantum Sieving of Hydrogen Isotopologues in Carbon Nanotubes: Competition of ZPE effects and Resonance Enhanced Tunneling (poster)*  
M. Mondelo-Martell, F. Huarte-Larrañaga

7th European Conference on Molecular Magnetism (ECMM 2019)  
Florence (Italy) 15-19 September 2019

*Magnetism and electronic transport in Bisdithiazolyl-based multifunctional materials: a computational study (poster)*  
C. Roncero

*Revising the common understanding of metamagnetism in the molecule-based bisdithiazolyl BDTMe compound (poster)*  
M. Deumal

*Encapsulating Mononuclear Single Molecule Magnets (oral communication)*  
S. Gómez-Coca, M. Amoza, L. Maxwell, E. Ruiz

European Materials Research Symposium Fall Meeting 2019 – Symposium Q  
Warsaw (Poland) 16 September 2019

*Breaking scaling relations does not always lead to enhanced OER electrocatalysts (invited talk)*  
Federico Calle-Vallejo
III. SCIENTIFIC ACTIVITY OF IQTCUB MEMBERS

*Tracking the Properties of Oxides from Nanoparticle to Bulk (oral communication)*
S. T. Bromley

*Understanding the Interplay between Size, Morphology and Energy Gap in Photoactive TiO₂ Nanoparticles (oral communication)*
S. T. Bromley

*Interplay between Size, Morphology and Energy Gap in Realistic TiO₂ Nanoparticles (oral communication)*
Á. Morales-García, A. Macià, S. T. Bromley, F. Illas

The 23rd International conference on “Horizons in Hydrogen Bond Research” (HBOND2019)
Amsterdam (Netherlands) 23 September 2019

*Non-terrar biosolvents model structure, stability and replication of B-DNA (invited talk)*
J. Poater, T.A. Hamlin, C. Fonseca Guerra, F.M. Bickelhaupt

XI International Conference on Mechanisms of Catalytic Reactions
Sochi (Russia) 7 – 11 October 2019

*K. M. Neyman (scientific committee and chairman scientific session)*

*Metal/metal-oxide interface effects in catalytic materials: Theory versus experiment (oral communication)*
K. M. Neyman

Blas Cabrera 2019 Physics Seminar
Tenerife (Spain) 16 October 2019

*Tailoring Low-Dimensional Materials with Impact on the Activation of CO₂ and on Photocatalysis (invited talk)*
Á. Morales-García
III. SCIENTIFIC ACTIVITY OF IQTCUB MEMBERS

22nd Conference on Process Integration for Energy Saving and Pollution Reduction - PRES’19
Creta (Greece) 20-23 October 2019

Integrated Reaction-Separation Processes Sequencing and Screening at Early Stages of Design (invited talk)

Hydration of Cyclohexene to Cyclohexanol In A Hybrid Reactive Distillation with A Side Decanter (poster)
I. Marchante, A. E. Plesu Popescu, V. Plesu, J. Bonet-Ruiz, P. Iancu, J. Llorens

Energy Consumption in Sharp and Non-Sharp Splits of Ideal Ternary Mixtures (poster)
S. Exposito, V. Plesu, J. Bonet-Ruiz, A. E. Plesu Popescu, P. Iancu, J. Llorens

Symposium “Advances in cluster beam deposition”
Okinawa (Japan) 20-25 November 2019

Metal/metal-oxide interface effects in catalytic nanomaterials: Theory versus experiment (oral communication)
K. M. Neyman

Brno (Czech Republic) 21-22 November 2019

Bioethanol dehydration process in a gasoline-mixing process (poster)
J. L. Pellín, A. E. Plesu, J. Bonet, J. Llorens

Concentration of orthophosphate and ammonium via forward osmosis to precipitate them as struvite (poster)
J. Labanda, J. Llorens, A. E. Plesu, J. Bonet

SancaMedChem2019 - The Sao Carlos Special Medicinal Chemistry Meeting
Sao Carlos (Brasil) 25-27 November 2019

Disclosing the molecular determinants of bioactive compounds: From chemical structure to mechanisms of drug action (oral communication)
F. J. Luque
Advances in Computational Biology (AdvCompBio 2019)
Barcelona (Spain) 28-29 November 2019

Model-driven discovery of metabolic reprogramming associated to metastatic cancer and cisplatin resistance (poster)
M. Cascante, C. Balcells, C. Foguet, M. Tarrado, O. Camacho, P. de Atauri, T. Thomson, F. Mas, S. Marin

Scientific Advisory Board Meeting of the IQTC-UB
Barcelona (Spain) 29 November 2019

Unravelling Calmodulin conformational ensemble from combined Molecular Dynamics and FRET simulations (poster)
D. Gonzalo, C. Curutchet

Dual classical/quantum MD strategy for the determination of site energies in photosynthetic complexes: Application to the PC645 antenna (poster)
B. Ozaydin, M. Corbella, C. Curutchet

First-Principles Evaluation of the Initial Oxidation of Transition Metal Surfaces (poster)
A. Jurado-Mañas, F. Viñes, F. Illas

Morphology Dependence of Stability and Properties of Stoichiometric TiO$_2$ Nanoparticles (poster)
Á. Morales-García, A. Macià, S. T. Bromley, F. Illas

H$_2$ Dissociation on Transition Metal Carbide Surfaces (poster)
J. J. Piñero, P. J. Ramírez, S. T. Bromley, F. Illas, F. Viñes, J. A. Rodríguez

Unraveling Morphological and Topological Key Aspects of Pd Nanoparticles (poster)
L. Vega, F. Viñes, K. M. Neyman

Accuracy of the Topological Approach for Nanoalloys: Case Study of PtCu Nanoparticles (poster)
L. Vega, F. Viñes, K. M. Neyman

X-Ray Photoelectron Spectroscopy: Theoretical Approach (poster)
M. Figueras, I. J. V. Garcia, F. Viñes, C. Sousa, V. A. de la Peña O’Shea, F. Illas

Tuning Activity of Transition Metal Carbides by Surface Metal Alloying: Case of Study of CO$_2$ Capture (poster)
M. López, L. Broderick, J. Carey, F. Viñes, M. Nolan, F. Illas

Subsurface Carbon: A General Feature of Noble Metals (poster)
O. Piqué, I. Z. Koleva, F. Viñes, H. A. Aleksandrov, G. N. Vayssilov, F. Illas
Grazynes: A New Family of Carbon-Based Materials from IQTCUB (poster)
P. Gamallo, F. Viñes

$CO_2$ Methanation Reaction on the Ni(111) Surface: First-Principles Kinetic Monte Carlo Study (poster)
P. Lozano, H. Prats, P. Gamallo, F. Illas, R. Sayós

Weak Polyelectrolyte Modelling: Coupling Charge Regulation and Conformational Equilibria vis LEIP Methodology (poster)
J. L. Garcés, P. M. Blanco, S. Madurga, F. Mas

A New Model for Macromolecular Diffusion in Crowded Media: the Chain Entanglement Soft Potential (poster)
P. M. Blanco, S. Madurga, J. L. Garcés, F. Mas

Effect of pH on conformational behaviour in peptides. Simulation of polyaspartic acid (poster)
C. Privat, S. Madurga, F. Mas, J. Rubio.

Analysis of the supramolecular structure of helicobacter pyloriurease extracellular at different pHs by molecular dynamics simulation (poster)
H. L. Barazorda-Ccahuana, B. Gómez, F. Mas, S. Madurga

Prediction of partition coefficients by ab initio calculations (poster)
L. Saranjan, M. Nedyalkova, V. Simeonov, F. Mas, S. Madurga

3rd International Caparica Christmas Conference on Translational Chemistry 2019
Lisbon (Portugal) 2 December 2019

Open-shell Jellium aromaticity in metal clústers (invited talk)
J. Poater, M. Solà

3rd International Caparica Christmas Conference on Translational Chemistry (IC3TC)
Caparica (Portugal) 2-5 December 2019

Molecular Magnetism: Tailoring Mononuclear Single Molecule Magnets behaviour of First-Row Transition Metal Complexes (comunicació oral)
S. Gómez-Coca, E. Ruiz
### RESEARCH STAYS IN RECOGNIZED CENTERS

<table>
<thead>
<tr>
<th>Name</th>
<th>Institution</th>
<th>Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alemany, P.</td>
<td><em>Universidad Católica del Norte</em> (Chile)</td>
<td>UB visiting researcher invited by Jaime Llanos. May 2019</td>
</tr>
<tr>
<td>Alemany, P.</td>
<td><em>Donostia International Physics Center, Donostia</em> (Spain)</td>
<td>UB visiting researcher invited by Abel Carreras. December 2019</td>
</tr>
<tr>
<td>Bernuz, E.</td>
<td><em>Donostia International Physics Center, Donostia</em> (Spain)</td>
<td>UB visiting researcher invited by Abel Carreras. December 2019</td>
</tr>
<tr>
<td>Curutchet, C.</td>
<td><em>Universitat Federal d'ABC, Santo André</em> (Brasil)</td>
<td>Research stay with Prof. Paula Homem-de-Mello. September 2019</td>
</tr>
<tr>
<td>Ginex, T.</td>
<td><em>University of Bristol, Bristol</em> (United Kingdom)</td>
<td>Research stay with Prof. Adrian Mulholland. February 2019</td>
</tr>
<tr>
<td>Llunell, M.</td>
<td><em>Donostia International Physics Center, Donostia</em> (Spain)</td>
<td>UB visiting researcher invited by Abel Carreras. December 2019</td>
</tr>
<tr>
<td>Neyman, K. M.</td>
<td><em>University of Sofia, Sofia</em> (Bulgaria)</td>
<td>Invited visiting researcher. May 2019</td>
</tr>
<tr>
<td>Nin-Hill, A.</td>
<td><em>University of York, York</em> (United Kingdom)</td>
<td>Research stay with Prof. Gideon J. Davies. April-June 2019</td>
</tr>
<tr>
<td>Rovira, C.</td>
<td><em>University of York, York</em> (United Kingdom)</td>
<td>Research stay with Prof. Gideon J. Davies. May-October 2019</td>
</tr>
</tbody>
</table>
PARTICIPATION IN COMPETITIVE FUNDED RESEARCH PROJECTS

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

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

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

Diseño Racional de Nuevos Catalizadores Heterogeneos, Electrocatalizadores y Fotocatalizadores Para la Produccion de Energía Limpia Sostenible a Traves de la Conversion de H₂.
F. Illas, University of Barcelona
RTI2018-095460-B-I00/AEI/FEDER, 2019 – 2021
Ministry of Economy and Competitiveness (MINECO)
Amount: 229.900 EUR

Química Computacional Aplicada para la captura, separación y conversión de CO₂ en combustibles ligeros.
R. Sayós, P. Gamallo, University of Barcelona
RTI2018-094757-B-I00/AEI/FEDER, 2019 – 2021
Ministry of Economy and Competitiveness (MINECO)
Amount: 85.426 EUR

Modeling and Simulation of reactive processes in enzymes by means of ab initio molecular dynamics and QM/MM methods.
C. Rovira, University of Barcelona
CTQ2017-85496-P/AEI/FEDER, 2018-2020
Ministry of Economy and Competitiveness (MINECO)
III. SCIENTIFIC ACTIVITY OF IQTCUB MEMBERS

_Diseño racional desde una perspectiva computacional de materiales basados en radicales orgánicos con propiedades de interés tecnológico._
M. Deumal, J. J. Novoa, University of Barcelona  
**CTQ2017-87773-P/AEI/FEDER, 2018-2020**  
Ministry of Economy and Competitiveness (MINECO)

_Structure-based modeling of the role of the environment in photosynthetic light harvesting and protein fluorescence._
C. Curutchet, University of Barcelona  
**CTQ2017-89924-P/AEI/FEDER, 2018-2020**  
Ministry of Economy and Competitiveness (MINECO)  
Amount: 65.340 EUR

_Estudio Computacional del Control Mecanoquímico de Reacciones de Interés en Química Biorgánica._
J. M. Bofill, I. de P. R. Moreira, University of Barcelona  
**CTQ2016-76423-P/AEI/FEDER, 2017-2019**  
Ministry of Economy and Competitiveness (MINECO)  
Amount: 36.300 EUR

_Diseño computacional de pares de bases de ADN artificiales que pueden ser replicados._
J. Poater, University of Barcelona  
**CTQ2016-77558-R/AEI/FEDER, 2016-2019**  
Ministry of Economy and Competitiveness (MINECO)

_Producción de bio-plásticos a partir de la fracción orgánica de residuos municipales._
J. Mata, J. Llorens, University of Barcelona  
**CTM2016-76275-R, 2016-2020**  
Ministry of Economy and Competitiveness (MINECO)  
Amount: 139.150 EUR

_Understanding, controlling and optimizing heterogeneous catalysts and photocatalysts at the nanoscale. Application to carbon dioxide conversion and hydrogen production._
F. Illas, S. T. Bromley, University of Barcelona  
**CTQ2015-64618-R/AEI/FEDER, 2016-2019**  
Ministry of Economy and Competitiveness (MINECO)

_Computational Materials Science Laboratory._
F. Illas, University of Barcelona  
**2017 SGR 13, 2018-2021**  
University and Research Grants Management Agency (AGAUR)  
Amount: 68.000 EUR
**III. SCIENTIFIC ACTIVITY OF IQTCUB MEMBERS**

*Modelització i Disseny de Sistemes Químics Radicalaris.*
J. M. Bofill, University of Barcelona

**2017 SGR 348, 2018-2020**
University and Research Grants Management Agency (AGAUR)
Amount: 20,000 EUR

*Grup de Bioinformàtica Integrativa.*
M. Cascante, University of Barcelona

**2017 SGR 1033, 2017-2020**
University and Research Grants Management Agency (AGAUR)

*Grup de recerca consolidat: Estructura i funció en macromolècules.*
C. Rovira, University of Barcelona

**2017 SGR 1189, 2017-2020**
University and Research Grants Management Agency (AGAUR)

*Grup d'Estructura Electrònica.*
S. Alvarez, University of Barcelona

**2017 SGR 1289, 2017-2019**
University and Research Grants Management Agency (AGAUR)
Amount: 44,480 EUR

*Biològia Computacional i Disseny de Fàrmacs.*
F. J. Luque, University of Barcelona

**2017 SGR 1746, 2017-2020**
University and Research Grants Management Agency (AGAUR)

*Theoretical study on the receptor-cannabinoid affinities and dynamics.*
C. Curutchet, University of Barcelona

**2018 DI 043, 2019-2021**
Catalan Government (GENCAT)
Amount: 21,600 EUR

*Beca Postdoctoral Beatriu de Pinós.*
Silvia Gómez-Coca, University of Barcelona

**2017 BP 00080, 2018-2020**
Catalan Government (GENCAT)
Amount: 90,000 EUR
Captura de CO₂ emitido por vehículos basados en motores de combustión, mediante absorción en sólidos porosos.
X. Gimenez, P. Gamallo, University of Barcelona
IDI-20190124, 2019-2021
Center for Industrial Technological Development (CDTI), Recam Laser S.L.
Amount: 146,000 EUR

Deciphering the Metabolism of Haematological Cancers (HaemMetabolome).
M. Cascante, University of Barcelona
8P1MCA- H2020. PILLAR 1-EXCELLENT SCIENCE. MCA. Marie Sklodowska-Curie Actions, 675790, 2015-2019
European Union

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

Instituto Nacional de Bioinformática.
M. Cascante, University of Barcelona
Ayudas para proyectos de investigación del área de Ciencias de la Salud (FIS), 2018-2020
Ministry of Economy and Competitiveness (MINECO)

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

Recuperació i valorilzació de recursos de digestats urbans en el marc de l'economia circular (DIGESTAKE).
J. F. Garcia, University of Barcelona
COMRD16-1-0061-01, 2017 – 2020
Acció, Catalan Business Support Agency
Amount: 117,934 EUR

Energy and charge transfer by non-orthogonal configuration interaction
C. Sousa, M. Llunell, University of Barcelona
CHM154, 2019-2020
Oak Ridge Leadership Computing Facility (USA)
Mecanismos moleculares implicados en la inhibición de dianas para tratamientos anti-influenza: canal de protones M2 y hemaglutinina.
F. J. Luque, University of Barcelona
Ministry of Economy and Competitiveness (MINECO)
Amount: 90.750 EUR

Identificación, síntesis y evaluación toxicológica de molécula propia antidetonante.
F. J. Luque, University of Barcelona
FBG-309799, 2018-2019
REPSOL-YPF, SA
Amount: 98.780 EUR

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, University of Barcelona
European Union

QUIFIEXP - Quimica Fisica Experimental.
J. Ignes, University of Barcelona
GINDO-UB/112, 2016-2019
PPID – Teaching Innovation Projects (UB)

ICREA Acadèmia.
F. Illas, University of Barcelona
2016-2020
Catalan Institute for Advanced Research (ICREA, Generalitat de Catalunya)

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

COST Action CA18234 – Computational materials sciences for efficient water splitting with nanocrystals from abundant elements
M. Caspary Toroker, TECHNION, Haifa, Israel
European Commission, 2019-2023
European Cooperation in Science and Technology Program
Estudi de laboratori i planta pilot per la recuperació d’amoní dels purins.
J. Mata Álvarez, F. Mas, University of Barcelona
Private company contract, 2017-2019
INDUKERN (Veterinary division)

Reactivity of lattice oxygen in nanostructured CeO\textsubscript{2} doped by Pt and Pd.
K. Neyman, University of Barcelona
QCM-2018-3-0018, 2018-2019
Spanish Supercomputing Network (RES)

Atomic ordering in bimetallic nanoparticles of fcc-type: Pt-Ni.
K. Neyman, University of Barcelona
Spanish Supercomputing Network (RES)

Striking chemical orderings in bimetallic nanoparticles with silver and gold atomic shells.
K. Neyman, University of Barcelona
QS-2019-3-0023, 2019-2020
Spanish Supercomputing Network (RES)
Institut de Química Teòrica i Computacional