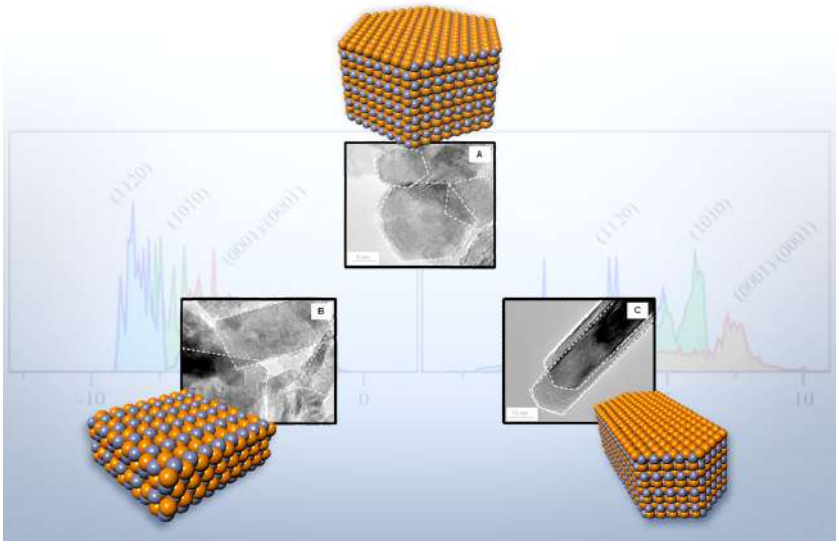
Institut de Química Teòrica i Computacional

Universitat de Barcelona

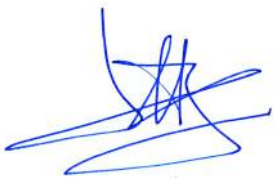
Institut de Química Teòrica i Computacional de la Universitat de Barcelona (IQTCUB)



Activity Report 2015

The creation of the Institute of Theoretical Chemistry of the *Universitat de Barcelona* (IQTCUB) was approved on November 27th, 2007. The members of IQTCUB are professors and researchers from different departments of the Chemistry and Physics faculties of UB who employ methods of Computational Chemistry and/or Computational Physics (e.g. Quantum Chemistry, Solid State Modeling). The IQTCUB research activity focuses mainly in the field of Chemistry. Yet, this activity is quite different from what one expects from a traditional chemist. Indeed, the instruments used by the IQTCUB members cannot be found in a typical chemical laboratory but rather in a virtual "computational laboratory" with supercomputers having hundreds or thousands of processors. The main goals of Theoretical and Computational Chemistry are: to achieve a detailed understanding of chemical process at the molecular level, to suggest new experiments by means of predictions that have to be experimentally proven, to interpret and provide a rationale of complex experimental results, and to devise new tools and concepts. Following these general objectives, the IQTCUB aims to design new materials and drug molecules with tailored properties, investigate new chemical reactions to obtain key products with improved efficiency and selectivity, to improve existing processes with respect to efficiency and environmental impact, and to propose new sources of sustainable energy. Although most of these goals are common to other scientific disciplines (given the interdisciplinary approach of modern research), the insights provided by theoretical and computational chemistry are unique and cannot be obtained with other methods. Therefore, the tools developed and employed in IQTCUB play a prime role in solving many pressing challenges faced by modern society.

Once again, this has been a difficult year with unprecedented cuts in the overall research budget of the whole country. Still, through the support of Research Vicerector, UB has renewed the compromise with the IQTCUB. This is fully acknowledged by all personnel of the institute who otherwise could not carry out this research. In fact, without the support from the institution it would be impossible to maintain the computational infrastructure, which is essential to carry out a high-quality and competitive research. This is also thanks to the, often invisible, excellent technical staff that is responsible for keeping the whole computational framework working. This *activity report* evidences the IQTCUB vitality, the considerable scientific production in research lines as diverse as drug design, heterogeneous catalysis, nanostructures, novel materials, and atmospheric chemistry clearly demonstrates the growing impact of our research. We do hope that the IQTCUB project will continue to deserve the support of our university in the years to come. This will certainly be essential to further improve the scientific quality of IQTCUB, which was already recognized by external peer review evaluation in 2013.



Francesc Illas
Director de l'IQTCUB

REPORT CONTENT

I. IQTCUB OVERVIEW

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

I.1 DIRECTION TEAM

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

I.2 IQTCUB RESEARCH LINES

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

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

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

2. **Computational Materials Science**

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

3. **Computational Biochemistry and Soft Matter**

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

4. **Reactivity and Reaction Dynamics**

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

I.3 IQTCUB MEMBERS

IQTCUB involves a total of 83 professors and researchers: The full list of members of IQTCUB (including the corresponding academic stuation and affiliation within UB) is provided below.

Family Name	Name	Department/Unit
Full Professors (Catedràtics)		
Aguilar Navarro	Antonio	Physical Chemistry
Alemany i Cahner	Pere	Physical Chemistry
Alvarez Reverter	Santiago	Inorganic Chemistry
Bofill Villà	Josep Maria	Organic Chemistry
González Pérez	Miguel	Physical Chemistry
Illas Riera	Francesc	Physical Chemistry
Mas Pujadas	Francesc	Physical Chemistry
Novoa Vide	Juan José	Physical Chemistry
Rubio Martínez	Jaime	Physical Chemistry
Ruiz Sabin	Eliseo	Inorganic Chemistry
Sayós Ortega	Ramón	Physical Chemistry
Associate Professors (Professors Titulars)		
Albertí Wirsing	Margarita	Physical Chemistry
Costa Sala	Ramón	Inorganic Chemistry
De Andrés Llopis	Jaime	Physical Chemistry
De Pinho Ribeiro Moreira	Ibério	Physical Chemistry
Giménez Font	Xavier	Physical Chemistry
Huarte Larrañaga	Fermín	Physical Chemistry
Lucas Alcorta	Josep Maria	Physical Chemistry
Llunell Marí	Miquel	Physical Chemistry
Mota Valeri	Fernando	Physical Chemistry
Paniagua Valle	Juan Carlos	Physical Chemistry
Solé Sabaté	Albert	Physical Chemistry
Sousa Romero	Carme	Physical Chemistry
Vilaseca Font	Eudald	Physical Chemistry

Other categories (Professors Agregats i Lectors)

Aullón López	Gabriel	Inorganic Chemistry
Deumal Solé	Mercè	Physical Chemistry
Gamallo Belmonte	Pablo	Physical Chemistry
Madurga Díez	Sergio	Physical Chemistry
Ribas Ariño	Jordi	Physical Chemistry
Reigada Sanz	Ramón	Physical Chemistry

Other categories (Professors Associats)

Gómez Coca	Silvia	Inorganic Chemistry
Jover Modrego	Jesús	Inorganic Chemistry
Tercero Mohedano	Javier	Inorganic Chemistry

ICREA Research Professors

Bromley	Stefan T.	Physical Chemistry
Neyman	Konstantin M.	Physical Chemistry
Rovira Virgili	Carme	Organic Chemistry

Postdoctoral contracts

Beatriu de Pinós-Marie Curie

Cirera Fernández	Jordi	Inorganic Chemistry
Echeverría López	Jorge	Inorganic Chemistry

Beatriu de Pinós

Albareda Piquer	Guillem	IQTCUB
Jornet Somoza	Joaquim	Physical Chemistry

Ramón y Cajal contract

Viñes Solana	Francesc	Physical Chemistry

Other

Alfonso Prieto	Mercedes	Organic Chemistry
Álvarez Falcón	Leny	Physical Chemistry
Chul Ko	Kyoung	Physical Chemistry
Kovács	Gábor	Physical Chemistry
Kozlov	Sergey M.	Physical Chemistry
Valero	Rosendo	Physical Chemistry

Ph D students

FPI (Associated with Ministerio Research Grants)

Alonso Gil	Santiago	Organic Chemistry
Climent Biescas	Clàudia	Physical Chemistry
Falceto Palacín	Andrés	Inorganic Chemistry
Jurado Sáez	Manuel	Physical Chemistry
Posada Pérez	Sergio	Physical Chemistry
Vilà Casanova	Arnau	Physical Chemistry

FPU (Spanish Ministerio Program)

Alcon Rovira	Isaac	Physical Chemistry
Amoza Dávila	Martín	Inorganic Chemistry
Garrido Sagargazu	Eduardo	Physical Chemistry
Mondelo Martell	Manel	Physical Chemistry
Rojas Cervellera	Victor	Organic Chemistry

UB own program

Blancafort Jorquera	Miquel	Physical Chemistry
Fumanal Quintana	Maria	Physical Chemistry
Lamiel Garcia	J. Oriol	Physical Chemistry
Raich Armendáriz	Lluís	Organic Chemistry

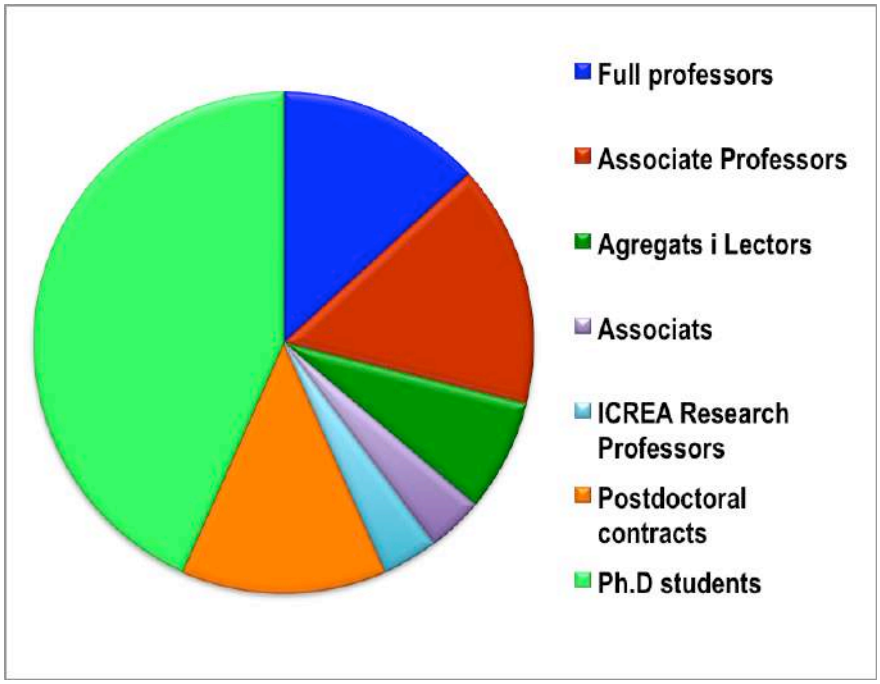
FI (Catalan Government Program)

López Marne	Estefanía	Physical Chemistry
Prats García	Hèctor	Physical Chemistry

Other funding

Alonso Benito	Gerard	Physical Chemistry
Balcells Nadal	Cristina	Physical Chemistry
Cebrián Prats	Anna	Physical Chemistry
Cuko	Andi	Physical Chemistry
Figueroba Sánchez	Alberto	Physical Chemistry
Francese	Tommaso	Physical Chemistry
Jiménez Grávalos	Fernando	Physical Chemistry
Macià Escatllar	Antoni	Physical Chemistry
Manadé Company	Montserrat	Physical Chemistry
Martín Rodríguez	Alejandro	Inorganic Chemistry
Maxwell Villacorta	Lindley	Inorganic Chemistry
Millán Alvares	Maria Angeles	Physical Chemistry
Muñoz Galán	Helena	Physical Chemistry
Notario Estévez	Almudena	Physical Chemistry
Omidvar	Akbar	Physical Chemistry
Pueyo Bellafont	Noelia	Physical Chemistry

Reta Mañeru	Daniel	Physical Chemistry
Roncero Barrero	Cristina	Physical Chemistry
Sopena Moros	Arturo	Physical Chemistry



Distribution of IQTCUB members according to professional category

I.4 TECHNICAL STAFF

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

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

I.5 EQUIPMENT

Currently, the IQTCUB computational facilities consist of seven calculation clusters located in two conditioned rooms of the Chemistry Faculty of UB. All the clusters except iqtc06 are located 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 is located in a room called VAX, which is cooled by an air conditioner machine of 30.000 KW and another two of 9.000KW.

CALCULATION CLUSTERS

cerqt2 (approximate value 400.000 €)

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

Specifications

Master
CPU: 1.80Ghz Opteron Dual processor (64bits)
RAM: 8GB
HD: 1x146GB hard disk + 2.5TB direct attached storage
Network: 2 gigabit network cards (one for external network and one for calculation network)

7 Sun Fire V60X nodes (3.06Ghz processor)
CPU: 3.06GHz Xeon Dual processor (32 bits)
RAM: 3GB
HD: 2x36GB hard disk
Network: 2 gigabit network cards (calculation network)

92 Sun Fire V60X nodes (2.80GHz processor)
CPU: 2.80GHz Xeon Dual processor (32 bits)
RAM: 6 nodes with 4GB, 86 nodes with 3GB
HD: 2x36GB hard disk
Network: 2 gigabit network cards (calculation network)

11 Sun Fire V20Z nodes (1.80GHz processor)
CPU: 1.80GHz Opteron Dual processor (64 bits)
RAM: 10 nodes with 8GB, 2 nodes with 16GB
HD: 10 nodes with 2x73GB hard disk, 2 nodes with 2x73GB and 2x300GB hard disk

respectively
Network: 2 gigabit network cards (calculation network)

1 Sun Fire V20Z node 64 bits (2.20GHz processor)
CPU: 2.20GHz Opteron Dual processor (64 bits)
RAM: 16GB
HD: 2x146GB hard disk
Network: 2 gigabit network cards (calculation network)

iqtc01 (approximate value 250.000 €)

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

80 AMD HP ProLiant DL145 G2 nodes
CPU: 2x2.2GHz AMD Opteron 275 Dualcore
RAM: 8GB
HD: 2x80GB hard disk
Network: 2 gigabit network card (calculation network) + 1 ILO card (out of band network, OOB)

iqtc02 (approximate value 78.000 €)

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

17 INTEL HP ProLiant DL160 G5 nodes
CPU: 2x2.66GHz Xeon QuadCore
RAM: 16GB
HD: 2x250GB hard disk
Network: 2 gigabit network card (calculation network) + 1 ILO card (OOB)

5 INTEL HP ProLiant DL160 G5 nodes
CPU: 2x2.66GHz Xeon QuadCore
RAM: 16GB
HD: 4x250GB hard disk
Network: 2 gigabit network card (calculation network) + 1 ILO card (OOB)

1 INTEL HP ProLiant DL160 G5 nodes
CPU: 2x2.66GHz Xeon QuadCore
RAM: 16GB

HD: 2x500GB hard disk
Network: 2 gigabit network card (calculation network) + 1 ILO card (OOB)

3 INTEL HP ProLiant DL160 G5 nodes
CPU: 2x2.66GHz Xeon QuadCore
RAM: 32GB
HD: 2x250GB hard disk
Network: 2 gigabit network card (calculation network) + 1 ILO card (OOB)

iqtc03 (approximate 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	

10 INTEL HP ProLiant DL140 G3 nodes
CPU: 2x2.33GHz Xeon QuadCore
RAM: 16GB
HD: 2x80GB hard disk
Network: 2 gigabit network card (calculation network) + 1 ILO card (OOB)

1 INTEL HP ProLiant DL140 G3 nodes
CPU: 2x2.33GHz Xeon QuadCore
RAM: 32GB
HD: 2x80GB hard disk
Network: 2 gigabit network card (calculation network) + 1 ILO card (OOB)

iqtc04 (approximate 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: 2x2.66GHz Xeon SixCore
RAM: 48GB
HD: 1x1TB 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: 2x2.66GHz Xeon SixCore

RAM: 48GB
HD: 4x500GB 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: 2x2.66GHz Xeon SixCore
RAM: 48GB
HD: 1x500GB hard disk
Network: 2 gigabit network card (internal data network and calculation network) + 1 ILO card (OOB)

iqtc05 (approximate value 32.000 €)

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

4 AMD SGI H2106-G7 nodes
CPU: 4x2.3GHz Opteron 6276 16-core
RAM: 256GB
HD: 2x1TB hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (OOB)

iqtc06 (approximate value 400.000 €)

Machine type	Heterogeneous Cluster
Operating System	SLES11
Services	Calculation cluster
Structure	28 nodes
Notes	64 bits processors
Specifications	

25 INTEL HP ProLiant DL560 Gen8 nodes
CPU: 4x2.2GHz Xeon OctoCore
RAM: 512GB
HD: 2x300GB hard disk
Network: 4 gigabit network card (calculation network) + 1 IPMI card (OOB)
Network: 2 10gigabit network card (internal data network)

6 INTEL Supermicro SuperServer 8017R-TF+
CPU: 4x2.3GHz Xeon OctoCore
RAM: 512GB
HD: 3x1TB hard disk

Network: 2 gigabit network card (calculation network) + 1 IPMI card (OOB)
Network: 2 10gigabit network card (internal data network)

GPU cluster (approximate value 35.000 €)

Machine type	Heterogeneous Cluster
Operating System	SLES11
Services	Calculation cluster with GPUs
Structure	4 nodes
Notes	64 bits processors
Specifications	

Node
CPU: 1x3.06GHz Intel Core i7 950
RAM: 16GB
HD: 1x1TB hard disk
Network: 1 gigabit network card (calculation network)
GPU: 1 NVIDIA GTX580, 1 NVIDIA GTX480

Node Tyan FT72B7015
CPU: 2x2.66GHz Xeon SixCore
RAM: 48GB
HD: 1x500GB hard disk
Network: 4 gigabit network card (calculation network) + 1 IPMI card (OOB)
GPU: 8 NVIDIA GTX580

Node
CPU: 1x3.30GHz AMD FX-4100 QuadCore
RAM: 16GB
HD: 1x1TB hard disk
Network: 1 gigabit network card (calculation network)
GPU: 1 NVIDIA GTX770

Node ASUS ESC4000 G2
CPU: 2x2GHz Xeon SixCore
RAM: 32GB
HD: 1x2TB hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (OOB)
GPU: 4 NVIDIA GTX TITAN

Node ASUS ESC4000 G2
CPU: 2x2.4GHz Xeon SixCore
RAM: 32GB
HD: 1x1TB hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (OOB)
GPU: 4 NVIDIA GTX TITAN BLACK

Node AZServer 4G3S
CPU: 2x2.4GHz Xeon E5-2620v3
RAM: 32GB
HD: 1x1TB hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (OOB)
GPU: 4 NVIDIA GTX 980

SERVERS

Glusterfs disk server (approximate value 30.000 €)

Machine type DELL cluster
Operating system SLES 11

Services Storage service cluster with 8TB of space for applications directories and user's work area exported by GlusterFS
Structure 2 nodes
Notes Storage service with a dedicated UPS and redundant power supply
Specifications

2 INTEL DELL PowerEdge 2950 nodes
CPU: 2x2.50GHz Xeon QuadCore E5420
RAM: 8GB
HD: 4x1TB (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: 2x2.27GHz Xeon QuadCore E5520
RAM: 56GB
HD: 12x2TB (raid 5)
Network: 2 gigabit network card (internal network) + 1 IPMI card (OOB)

1 INTEL HP ProLiant DL380e Gen8 node
CPU: 2x2.20GHz Xeon QuadCore E5-2407
RAM: 48GB
HD: 12x2TB (raid 5)

Network: 2 gigabit network card (internal network) + 1 IPMI card (OOB)

Portal (user access servers) (approximate value 2.300 €)

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

2 INTEL HP ProLiant DL120 G5 node
CPU: 1x2.33GHz Xeon Dual Core
RAM: 8GB
HD: 1x160GB hard disk
Network: 2 gigabit network card (internal network)

Virtualization servers (approximate value 18.300 €)

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

2 INTEL DELL PowerEdge 2950 nodes
CPU: 2x2.50GHz Xeon QuadCore E5420
RAM: 8GB
HD: 2x1TB (raid 1)
Network: 3 gigabit network card (internal network)

2 INTEL HP ProLiant DL120 G5 node
CPU: 1x2.33GHz Xeon Dual Core
RAM: 8GB
HD: 2x160GB hard disk
Network: 3 gigabit network cards (internal network)

Graphical applications server (approximated value 3.000 €)

Machine type	1 HP ProLiant DL385 node
Operating system	Debian Stable
Services	Server for the use of graphical applications (gaussview, p4vasp, etc.)

Structure	1 node
Notes	Server connected to an UPS
Specifications	
	1 AMD HP ProLiant DL385 node CPU : 2x2.2GHz AMD Opteron 275 Dualcore RAM: 4GB HD: 6x146GB hard disk Network: 1 10/100 network (external network) + 1 gigabit network (internal network)

OTHERS

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

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

The approximated total cost of this equipment is 50.000€

SUMMARY

Cores ..... 3326 CPUs

Memory.....23224 GB RAM

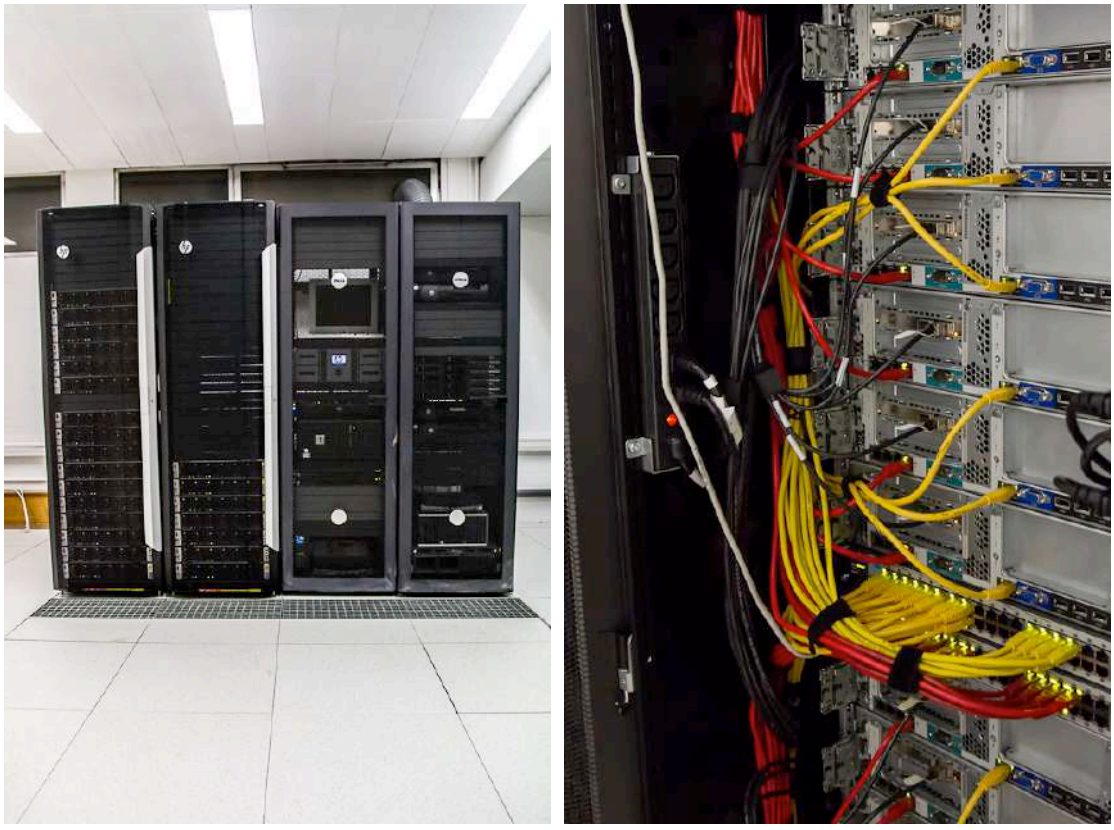
Calculation disk capacity ..... 176 TB

Data user disk capacity ..... 32 TB

The approximated total cost, considering also the consumables such as network cables and other material is

2.145.000 €*

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



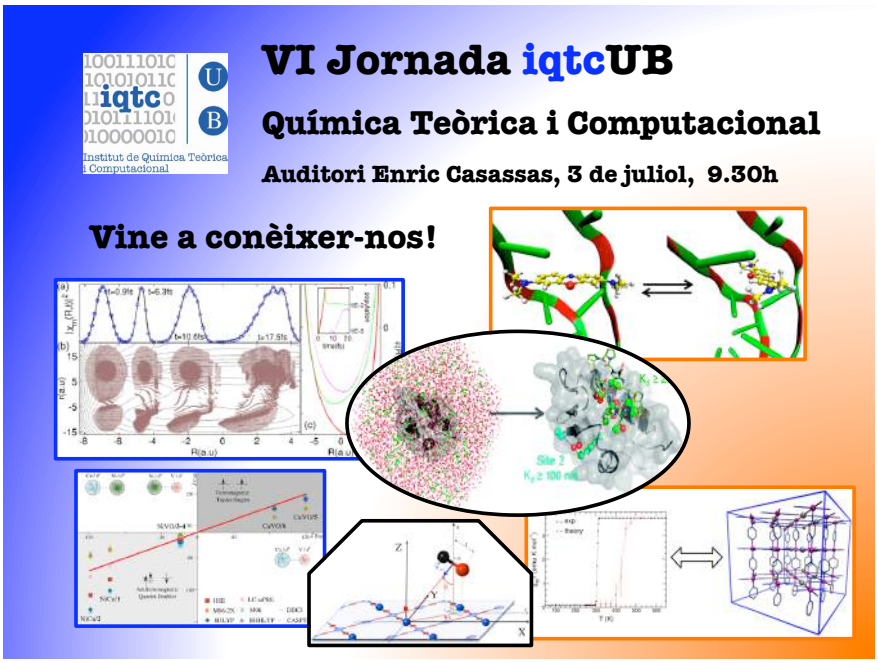
One of the clusters for intensive computation at IQTCUB

II. IQTCUB ACTIVITIES

II.1 GENERAL ACTIVITIES

Next, a description of activities and actions promoted by IQTCUB through 2015 is provided.

a. *6th IQTCUB workshop*. This one-day workshop aimed at the dissemination of the research done at the IQTCUB took place on July 3rd, 2015. The IQTCUB members and internationally acknowledged speakers present the most recent work. This year we highlight the participation of Prof. Leticia González from *University of Vienna,* and Dr. Guillem Albareda, Dr. Pablo Gamallo, Dr. Xavier Barril, Dr. Jordi Cirera, and Mr. Daniel Reta from Universitat de Barcelona. The IQTCUB assigned a budget to cover the traveling expenses of Prof. González as well as the catering service offered to all assistants. Total cost: 1040 €.



b. *Promotion and encouragement of research*. This year the IQTCUB has finally offered one contract (around 2000 € per contract) aimed to help students to initiate a scientific career. These contracts are addressed to students about to end the degree and aimed to cover a six month period to facilitate the student to pursue an official Master at UB as well as collaborating in some of the research projects of the IQTCUB groups. The contract has been awarded to Mr. Pablo Miguel Blanco Andrés. Total cost: 2000 €

c. *Introductory course in Computational Chemistry.* The main goal of this course is to initiate chemistry undergraduate students in the possibilities of Computational Chemistry. The course takes place during a whole week and is mainly addressed to Chemistry and Chemical Engineering students at the UB. The 2015 edition has been the fifth one and has been very successful with over 30 students requesting to participate. With respect to previous editions we have included a session oriented towards the visualization of biomolecules. Topics covered have been:

- Materials science
- Diffusion processes
- Molecular representation
- Visualization of biomolecules
- Advanced programming
- Advanced Linux

The course took place from June 25th to July 1st with an attendance of 25 students. IQTCUB has covered catering expenses with a total cost of 250 €.

d. Advanced Course in Computational Chemistry. Fuelled by the positive feedback received from the students in the previous editions we have offered again this year a course at a more advanced level with the main goal of improving previous knowledge in use of computers and, in particular, on Computational Chemistry. Participants in the course are usually students who have taken part in the introductory course or Chemistry undergraduates who have followed a Quantum Chemistry course. The course took place in July, 2st-9th with an attendance of 11 students. IQTCUB has covered catering expenses with a total cost of 240 €.

Picture corresponding to the "Advanced Course in Computational Chemistry" that took place in July 2015 at the Chemistry Faculty of the *Universitat de Barcelona*. Visit to Barcelona Supercomputer Center.

e. Intensive Course of the European Master on Theoretical Chemistry and Computational Modelling. This course took place at the University of Barcelona from January 11th to February 6th, with an attendance of 30 students from different Spanish universities. This course, which was coordinated by Prof. Ramón Sayós (an IQTCUB member), involved 21 lecturers (some of them being members of IQTCUB).

II.2 IQTCUB SEMINARS AND CONFERENCES

Nine seminars have been organized by IQTCUB during 2015.

1. **Prof. Luca Gavioli** (Universita Cattolica del Sacro Cuoro) Italy

   Synthesis of nanoparticles by non-thermal laser ablation and supersonic cluster beam deposition

   March 4th, 2015

2. **Prof. Frank Hagelberg** (East Tennessee State University) USA

   Novel Materials Based on Carbon Nanostructures

   March 9th, 2015

3. **Prof. Isabelle André** (Université de Toulouse) France

   The contribution of structural computational biology to the engineering of enzymes and the development of novel synthetic reactions

   March 27th, 2015

4. **Prof. Vladimír Sychrovský** (Institute of Organic Chemistry and Biochemistry) Czech Republic

   The catalytic mechanism of hOGG1 base-excision repair enzyme; the theoretical modeling of reaction channels and substrate activation

   May 27th, 2015

5. **Prof. Jen-Shiang K. Yu** (National Chio Tung University) Taiwan

   Electronic Structure of Open-Shell Tetrahedral $\{Fe(NO)_2\}9$ Complexes

   June 30th, 2015

6. **Prof. Markus Wilde** (University of Tokyo) Japan

   Hydrogen transportation across palladium surfaces: Mechanism, structure sensitivity, and control

   July 2nd, 2015

7. **Prof. Olga Lopez-Acevedo** (Aalto University) Finnland

   DNA Base Pairing by Noble Metals: Structure and Electronic Properties from Density Functional Theory

   July 16th, 2015

8. **Prof. Peter J. Reilly** (Iowa State University) USA

   The Wonderful Enzyme Zoo

   October 16th, 2015

9. **Prof. Vladimiro Mujica** (Arizona State University) USA

   Influence of Molecular Chirality in STM junctions and long-distance ET in biological systems

   November 30th, 2015

II.3 IQTCUB INVITED RESEARCHERS

During 2015, a total of nine researchers from all over the world have spent some time at the IQTCUB collaborating in different research projects.

1. **Prof. Boutheina Kerkeni** (visitor within a COST program)
   Sungkyunkwan University, South-Korea
   March-June, 2015

2. **MsC. Daeheum Cho** (invited visitor)
   Sungkyunkwan University, South-Korea
   March-June, 2015

3. **David Mora Fonz** (visitor within a COST program)
   University College London, UK
   June-July, 2015

4. **MsC. Sunkyong Kim** (invited visitor)
   Sungkyunkwan University, South-Korea
   June-September, 2015

5. **Prof. José Manuel Granadino Rodán** (invited visitor)
   Universitat de Jaén, Spain
   July-September, 2015

6. **Mr. Christian Kunkel** (invited visitor)
   University of Wurzburg, Germany
   July-September, 2015

7. **Prof. Hristiyan Aleksandrov** (invited visitor)
   University of Sofia, Bulgaria
   September, 2015

8. **Dr. Ali Abedi** (invited visitor)
   University of the Basque Country, Spain
   October, 2015

9. **Dr. Fatma Benyettou** (invited visitor)
   Centre Universitaire de Ain Témouchent, Algeria
   November, 2015

III. SCIENTIFIC ACTIVITY OF IQTCUB MEMBERS

III.1 HIGHLIGHTS FROM MOST RELEVANT RESULTS

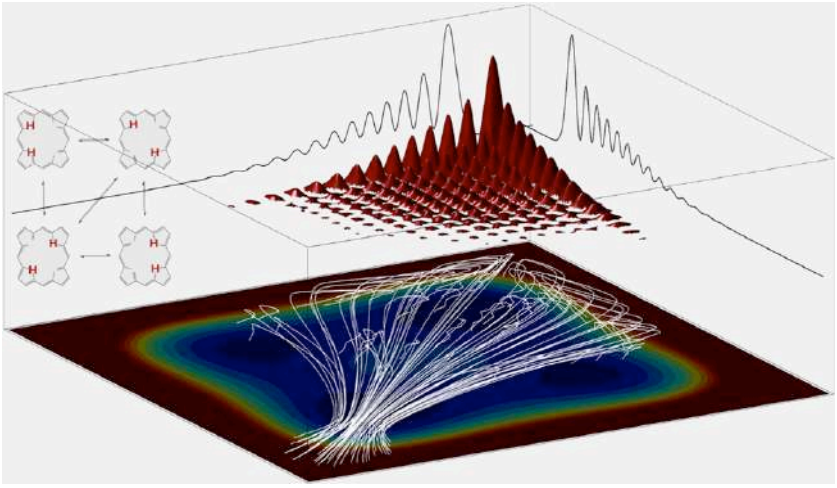
Here some of the most relevant results corresponding to every IQTCUB main research line are presented.

LINE 1. METHODS, ALGORITHMS AND COMPUTATIONAL TOOLS DEVELOPMENT

Conditional Born-Oppenheimer Dynamics: Quantum Dynamics Simulations for the Model Porphine

G. Albareda, J. M. Bofill, I. Tavernelli, F. Huarte-Larrañaga, F. Illas, A. Rubio.

J. Chem. Phys. Lett., *6* (2015) 1529.



Schematic representation of the conditional wave function concept for the model Porphine.

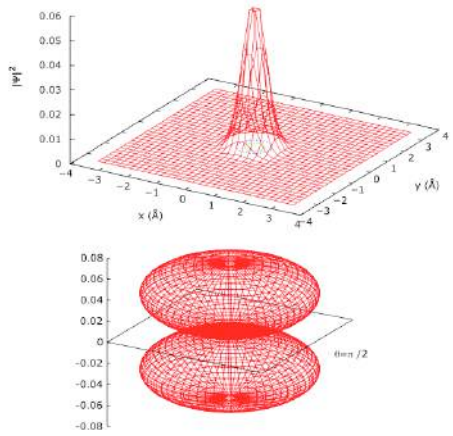
We report a new theoretical approach to solve adiabatic quantum molecular dynamics halfway between wave function and trajectory-based methods. The evolution of a N-body nuclear wave function moving on a 3N-dimensional Born−Oppenheimer potential-energy hyper-surface is rewritten in terms of single-nuclei wave functions evolving nonunitarily on a 3-dimensional potential-energy surface that depends parametrically on the configuration of an ensemble of generally defined trajectories. The scheme is exact and, together with the use of trajectory-based

statistical techniques, can be exploited to circumvent the calculation and storage of many-body quantities (e.g., wave function and potential-energy surface) whose size scales exponentially with the number of nuclear degrees of freedom. As a proof of concept, we present numerical simulations of a 2-dimensional model porphine where switching from concerted to sequential double proton transfer (and back) is induced quantum mechanically.

5D quantum dynamics of the H2@SWNT system: Quantitative study of the rotational- translational coupling

M. Mondelo-Martell, F. Huarte-Larrañaga.

J. Chem. Phys., *142* (2015) 084304.



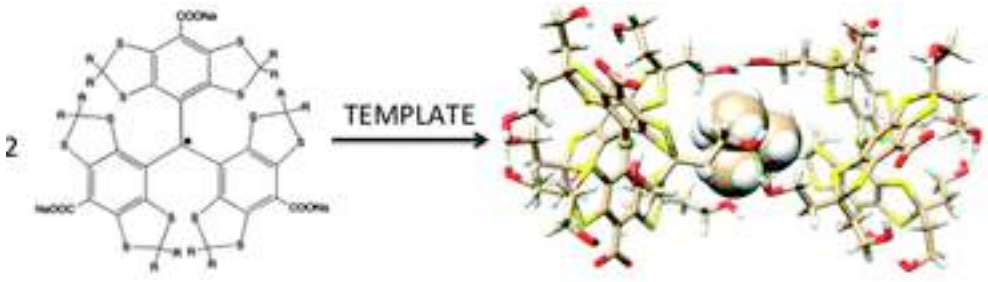
Groundstate of H_2 encapsulated in a (8,0) SWCNT. Translational (upper panel) and rotational (lower panel) functions.

The dynamics of the dihydrogen molecule when confined in carbon nanotubes with different chiralities and diameters are studied by using a 5 dimensional model considering the most relevant degrees of freedom of the system. The nuclear eigenstates are calculated for an (8,0) and a (5,0) carbon nanotubes by the State-Average Multiconfigurational Time-dependent Hartree, and then studied using qualitative tools (mapping of the total wave functions onto given subspaces) and more rigorous analysis (different kinds of overlaps with reference functions). The qualitative analysis is seen to fail due to a strong coupling between the internal and translational degrees of freedom. Using more accurate tools allows us to gain a deeper insight into the behaviour of confined species.

Self-assembled trityl radical capsules – implications for dynamic nuclear polarization.

I. Marin-Montesinos, J. C. Paniagua, M. Vilaseca, A. Urtizberea, F. Luis, M. Feliz, F. Lin, S. Van Doorslaerg and M. Pons.

Phys. Chem. Chem. Phys., *17* (2015) 5785.



Radical supramolecular capsules based on water soluble trityl.

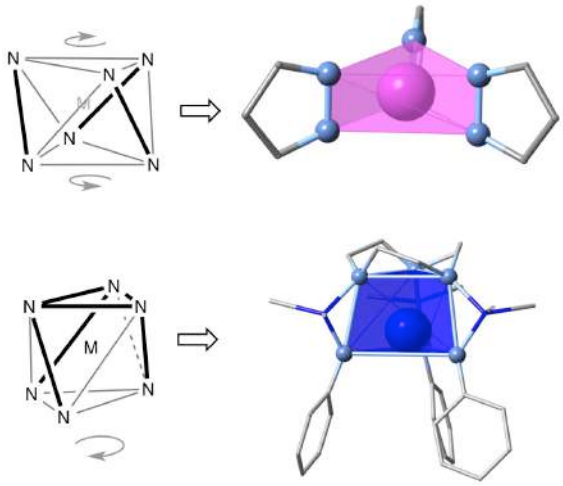
OX63 is a stable and water-soluble organic radical widely used in dynamic nuclear polarization (DNP). DFT calculations have shown that the molecule has a very stable dome-shaped conformation, and that two of these domes can be can be coupled together via three hydrogen bonds to form a sort of capsule, that can accommodate molecules as large as tetramethylammonium. This facts have a large impact on the behavior of OX63 in DNP, and allowed to explain several experimentally observed peculiarities.

LINE 2. COMPUTATIONAL MATERIALS SCIENCE

Distortion Pathways of Transition Metal Coordination Polyhedra Induced by Chelating Topology

S. Alvarez.

Chem. Rev., published ASAP (2015). Doi: 10.1021/acs.chemrev.5b00537

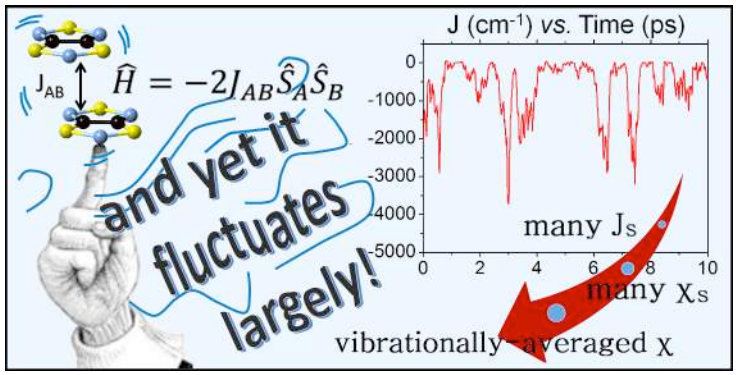


A continuous shape measures analysis of the coordination polyhedra of a host of transition metal complexes with bi- and multidentate ligands discloses the distortion pathway associated with each particular topology of the chelate rings formed. Since the degree of distortion within each family of complexes depends on the atomic size, on which the high- or low-spin state has a large effect, the analysis presented is specially interesting to identify distortions that go along with the transition from low to high spin state affected by temperature, light or pressure. Deviations from the expected distortion pathways in the high spin state are shown to be associated to the onset of intermolecular interactions such as secondary coordination of counterions or solvent molecules. Also significant displacement of counterions in an extended solid may result from the changes in metal-ligand bond distances when ligands are involved in intermolecular hydrogen bonding.

Dynamical effects on the magnetic properties of dithiazolyl bistable materials

S. Vela, M. Deumal, M. Shiga, J.J. Novoa, J. Ribas-Arino

Chem. Sci. *6* (2015) 2371.

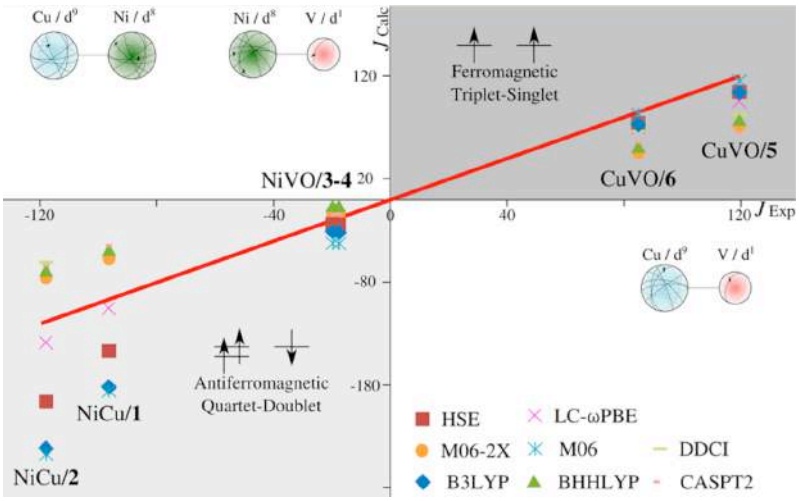


The magnetic properties of molecule-based magnets are commonly rationalized by considering only a single nuclear configuration of the system under study (usually an X-ray crystal structure). In this computational work, we have compared the results obtained using such a static approach with those obtained by explicitly accounting for thermal fluctuations, and uncovered the serious limitations of the static perspective when dealing with magnetic crystals whose radicals undergo wide-amplitude motions. As a proof of concept, these limitations heve been illustrated for the magnetically bistable 1,3,5-trithia-2,4,6-triazapentalenyl (TTTA) material. For its high-temperature phase at 300 K, we have shown that nuclear dynamics induce large fluctuations in the magnetic exchange interactions (J_{AB}) between spins (up to 1000% of the average value). These deviations result in a ~20% difference between the 300 K magnetic susceptibility computed by explicitly considering the nuclear dynamics and that computed using the X-ray structure, the former being in better agreement with the experimental data. The unveiled strong coupling between J_{AB} interactions and intermolecular vibrations reveals that considering J_{AB} as a constant value at a given temperature (as always done in molecular magnetism) leads to a flawed description of the magnetism of TTTA. Instead, the physically relevant concept in this case is the statistical distribution of J_{AB} values. The discovery that a single X-ray structure is not adequate enough to interpret the magnetic properties of TTTA is also expected to be decisive in other organic magnets with dominant exchange interactions propagating through labile π-π networks.

Spin Adapted Versus Broken Symmetry Approaches in the Description of Magnetic Coupling in Heterodinuclear Complexes

R. Costa, R. Valero, D. Reta-Mañeru, I. de P.R. Moreira, F. Illas.

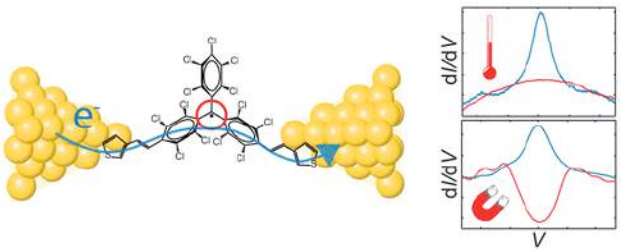
J. Chem. Theo. Comput. *11* (2015) 1006.



We have studied the performance of a series of multi-reference wave function and density functional theory based methods in predicting the magnetic coupling constants of heterodinuclear magnetic complexes. When using MR-WF methods the performance is found to be similar to other simple cases involving homodinuclear Cu(II) complexes, being the accuracy limited by the amount of dynamical correlation accounted for. When using DFT based methods, the usual broken symmetry approach provides a convenient framework to predict the magnetic coupling constants, although spin projection based techniques cannot recover the corresponding spin adapted solution. We have shown that a mapping procedure using the expectation values of the Heisenberg Hamiltonian in combination with a careful selection of the appropriate broken symmetry determinants provides a consistent relationship to derive J values from the BS solutions. Our trials using spin flip techniques lead to unphysical outcomes.

Kondo Effect in a Neutral and Stable All Organic Radical Single Molecule Break Junction

R. Frisenda, R. Gaudenzi, C. Franco, M. Mas-Torrent, C. Rovira, J. Veciana, I. Alcon, S. T. Bromley, E. Burzurí, H. S. J. van der Zant
Nano Letters *15* (2015) 310.



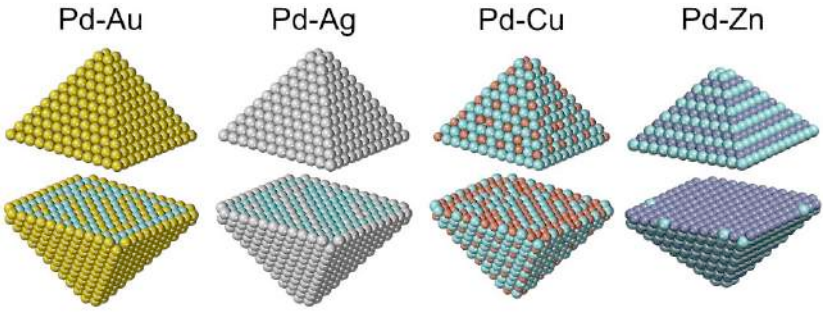
Kondo effect in an organic radical molecular junction

Experiments and computational modelling confirm the existence of the Kondo effect in an organic radical in a single molecule junction.

How to determine accurate chemical ordering in several nanometer large bimetallic crystallites from electronic structure calculations

S.M. Kozlov, G. Kovács, R. Ferrando, K.M. Neyman

Chem. Sci., *6* (2015) 3868.



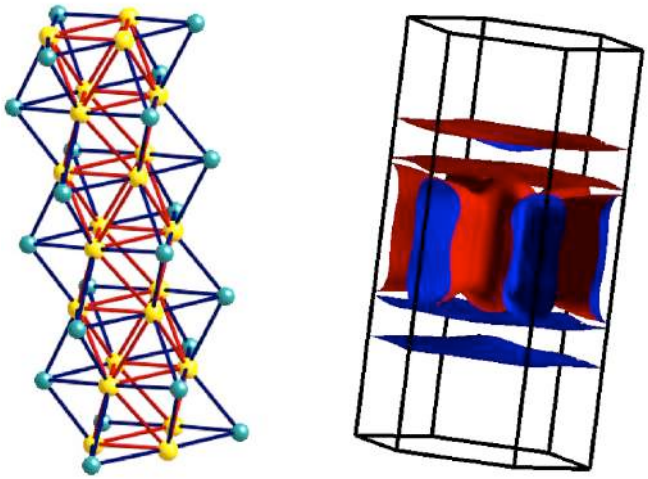
4.4 nm nanoparticles composed of >1400 atoms

Nanoalloys have a new degree of freedom compared to monometallic particles - the chemical ordering (COR) - the pattern, in which different atoms are located in the particle. The COR defines surface reactivity of nanoalloys. Experimental determination of the COR in bimetallic particles is very laborious. Also, calculation of the COR is a great challenge due to enormous number of possible mutual atomic positions in nanoparticles. We proposed an innovative method to accurately ascertain the COR using results of only several density functional calculations. This method immediately reveals why a certain COR is preferred. We unravelled the COR and binding nature in $Pd_{70}Au_{70}$, $Pd_{70}Ag_{70}$, $Pd_{70}Cu_{70}$ and $Pd_{70}Zn_{70}$ nanoparticles. The power of the method is also illustrated by optimizing the COR in larger $Pd_{732}Au_{731}$, $Pd_{732}Ag_{731}$, $Pd_{732}Cu_{731}$ and $Pd_{732}Zn_{731}$ particles, whose size ~4.4 nm is common in catalytic applications.

Links between the crystal and electronic structure in the new family of unconventional superconductors $A_2Cr_3As_3$ (A = K, Rb, Cs)

P. Alemany, E. Canadell

Inorg. Chem. *54* (2015) 8029.



Structure for a $[Cr_3As_3]^-$ chain (left) and Fermi surface (right) of the new low-dimensional $K_2Cr_3As_3$ superconductor

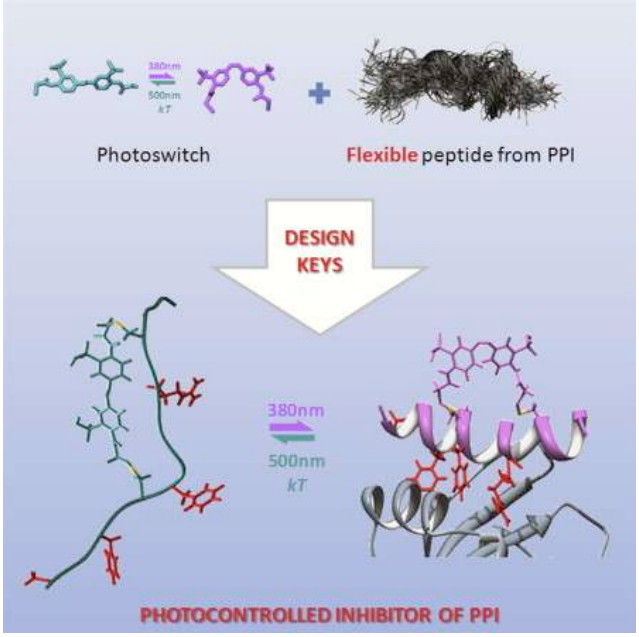
The electronic structure of a new family of superconductors is examined through density functional theory calculations. In contrast with other quasi-1D superconductors, these phases exhibit a relatively complex electronic structure and the Fermi surface contains both 1D and 3D components. It is shown that cations have an almost nil influence on the electronic structure. The absence of a structural Peierls modulation is discussed, and the differences with the structurally related $M_2Mo_6Se_6$ (M = Tl, In, ...) superconductors are stressed. The large electron mass renormalization and the lack of clear correlation between $N(e_F)$ and T_c suggest the existence of strong electron correlations and an unconventional origin of the superconductivity.

LINE 3. COMPUTATIONAL BIOCHEMISTRY AND *SOFT MATTER*

Absence of a Stable Secondary Structure Is Not a Limitation for Photoswitchable Inhibitors of βArrestin/ βAdaptin 2 ProteinProtein Interaction

A. Martín-Quirós, L. Nevola, K. Eckelt, S. Madurga, P. Gorostiza, E. Giralt.

Chemistry & Biology, *22* (2015) 31.



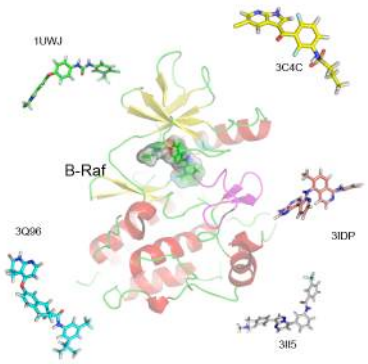
Design of a flexible photoswitchable inhibitor.

Many protein-protein interactions (PPIs) are mediated by short, often helical, linear peptides. Molecules mimicking these peptides have been used to inhibit their PPIs. Recently, photoswitchable peptides with little secondary structure have been developed as modulators of clathrin-mediated endocytosis. Here we perform a systematic analysis of a series of azobenzene-crosslinked peptides based to assess the relevance of secondary structure in their interaction with β-adaptin 2 and to identify photoswitchable inhibitors. We observe that flexible structures show a greater inhibitory capacity and enhanced photoswitching ability and that the absence of helical structures in free inhibitor peptide is not a limitation for their capacity. Therefore, our designed inhibitors expand the field of potential inhibitors of PPIs to the wide group of flexible peptides, and we argue against using a stable secondary structure as a sole criterion when designing PIPPI candidates.

Insight into the Binding of DFG-out Allosteric Inhibitors to B-Raf Kinase Using Molecular Dynamics and Free Energy Calculations

L. Coronel, JM, Granadino-Roldán, M. Pinto, MS. Tomas, MD. Pujol, J. Rubio-Martinez.

Current Computer-Aided Drug Design. *11* (2015) 124.



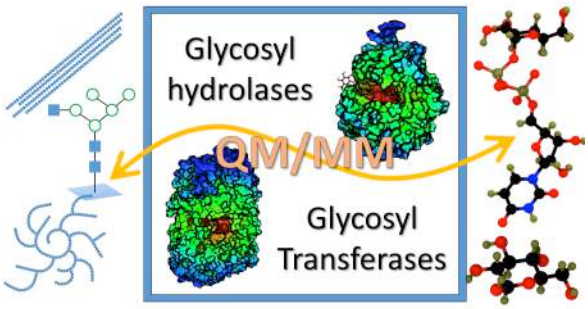
Interaction of B-Raf with some inhibitors

In this work, the energetics and structural keys of the binding of five different inhibitors to the oncogenic protein ^{V600EB}-Raf in its DFG-out conformation have been studied using MD and free energy calculations. The results obtained show that the binding free energy of these complexes is due to the individual contribution of many residues distributed throughout the binding site of the protein.

Reaction mechanisms in carbohydrate-active enzymes: glycoside hydrolases and glycosyltransferases. Insights from *ab initio* QM/MM dynamic simulations

A. Ardèvol, C. Rovira

J. Am. Chem. Soc., *137* (2015) 7528 (Perspective). Editor's choice & JACS Spotlight.



Carbohydrates are critical macromolecules in biochemistry and cell biology, notably in immunity and intercellular communication. Enzymes that help build, degrade, and modify these sugars are attractive targets for drug development, and also find major use in industrial biotechnology. But carbohydrates are often highly complex and flexible structures, ones that are synthetically challenging, and studying their intimate chemistry has proved difficult. In this Perspective, we review new molecular dynamics simulations using quantum mechanics and molecular mechanics (QM/MM) techniques that have fostered understanding of the mechanisms and conformational dynamics of two important classes of carbohydrate-active enzymes in the past decade. The two classes, glycosyl hydrolases and glycosyltransferases, catalyze the hydrolysis and synthesis, respectively, of glycosidic bonds between carbohydrates and their partner molecules. The results of the QM/MM simulations have fueled ongoing debate over which of several proposed mechanisms these enzymes follow.

Chloroform alters interleaflet coupling in lipid bilayers: an entropic mechanism

R. Reigada, F. Sagués.

J. R. Soc. Interface, *12* (2015) 20150197.

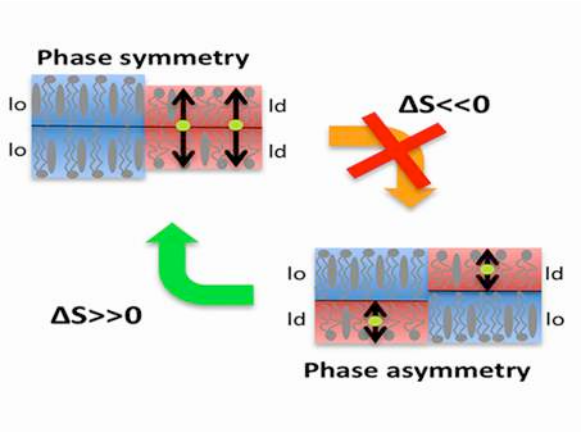


Illustration of the entropic linking mechanism that explains the interleaflet coupling effect of chlf molecules (green) in phase separating lipid bilayers. Double-tailed lipids and chol are shown schematically in grey ordered domains are plotted in red shading and disordered domains in blue shading.

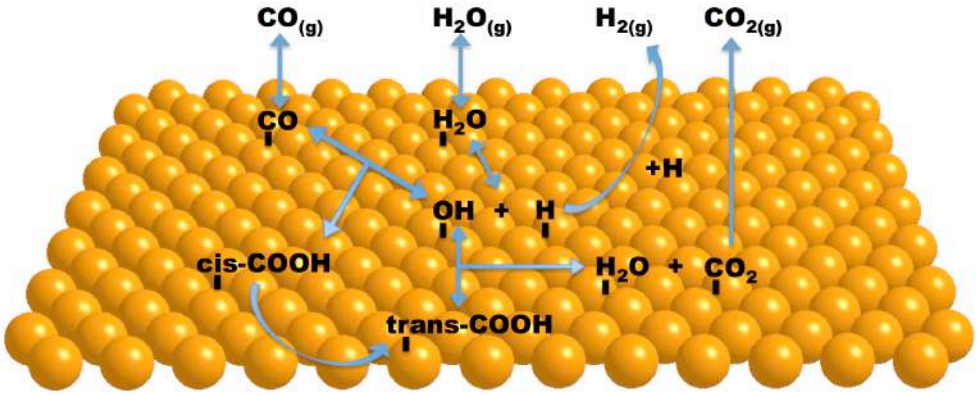
The molecular mechanism of general anesthesia is an unresolved issue. Some proposals suggest that the anesthetic compound changes the phasic state of the cell membrane. By means of molecular simulations we have unveiled that chloroform increases interleaflet interaction and promotes phase symmetry between membrane leaflets. This effect is due to an entropic mechanism that tries to avoid chloroform confinement to one of the leaflets. The reported effect and its consequences in transmembrane lipid distribution, cholesterol flip-flop, membrane curvature and mechanical properties is of interest for the understanding of the consequences of adding chloroform in cellular functions and its anesthetic effect.

LINE 4. REACTIVITY AND REACTIONS DYNAMICS

Kinetic Monte Carlo simulations of the water gas shift reaction on Cu(111) from density functional theory based calculations

H.Prats, L. Álvarez, F. Illas, R.Sayós

Journal of Catalysis (2015) (In press)

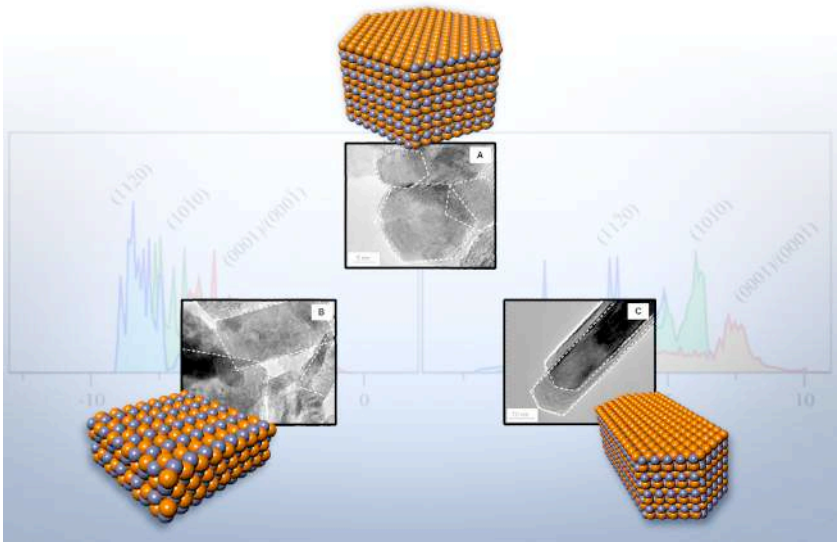


A systematic first-principles kinetic Monte Carlo study of the water gas shift reaction taking place on the Cu(111) surface is presented including adsorption/desorption, diffusion and other elementary chemical reactions, totalling 34 elementary steps with all reaction rates obtained from periodic density functional theory based calculations. The kinetic Monte Carlo simulations were carried out at different partial pressures and temperatures. The results show that the diffusion processes cannot be neglected and that the reaction proceeds predominantly through an associative mechanism via a carboxyl intermediate. The analysis of temperature dependence shows an Arrhenius behaviour with an apparent activation energy of 0.5-0.8 eV in agreement with experiments and with previous microkinetic studies. The effect of H_2O/CO ratio on this reaction shows that mixtures with higher CO proportion enhance the reactivity, also in accordance to previous studies. The present work allows one to ascertain the relative importance of the different steps in the mechanism of water gas shift reaction over Cu(111) at several conditions as well as to see the coverage evolution of the surface.

Morphology Effects in Photoactive ZnO Nanostructures: Photooxidative Activity of Polar Surfaces.

A. Iglesias-Juez, F. Viñes, O. Lamiel-Garcia, M. Fernández-García, F. Illas.

J. Mater. Chem. A *3* (2015) 8782.

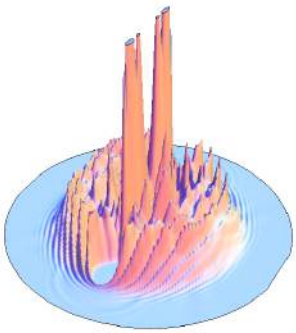


ZnO nanostructures with variable morphology were prepared by a microemulsion method and their structural, morphological, and electronic properties investigated by experimental and theoretical approaches using microscopy (high resolution transmission electron microscopy) and spectroscopic (X-ray diffraction, Raman, and UV-visible) tools, together with density functional theory calculations. Results provide a detailed insight into the relationship between surface-related physicochemical properties and the photochemical response of ZnO nanostructures, such as that the light-triggered photochemical activity of ZnO nanostructures is related to the predominance of highly-active (polar) surfaces, in particular, the amount of Zn-terminated (0001) surfaces, rather than band gap sizes, carrier mobilities, and other variables usually mentioned in the literature. The computational results highlight the oxidative capability of polar surfaces, independently of the degree of hydration.

Photodissociation dynamics of homonuclear diatomic molecules in helium nanodroplets. The case of $Cl_2@(^4He)_N$.

A. Vilà, M. González, R. Mayol.

J. Chem. Theory Comput., *11* (2015) 899.



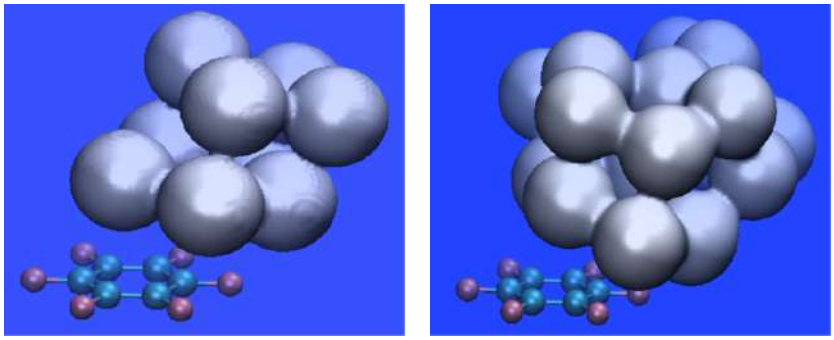
Snapshot showing the helium density (xz plane) close to the final of the $[Cl_2(B)@(^4He)_{500}]^*$ photodissociation process.

A hybrid method based on TDDFT (helium) and quantum dynamics (molecule) was developed to investigate the photodissociation of diatomic homonuclear molecules in superfluid ^{4}He nanodroplets (ND), T=0.37 K, allowing for the first time to study this important type of process. In the first application of this method the $Cl_2(B\leftarrow X)$ photodissociation for $Cl_2(v$=0,X)@$(^4He)_N$ nanodroplets with N=50-500 was examined. A time scale of a few ps was found for this process and at the high velocities involved an efficient energy exchange between the Cl atoms and the ND occurs, releasing up to 91% of the molecular energy (N=500). Moreover, the strongly oscillating final velocity distribution of the Cl dissociating atoms observed was due to the existence of confinement quantum interferences. As far as we know this is the first time that this type of interferences is described in the reaction dynamics context. We hope that these results will encourage the experimentalists to investigate these interesting systems.

A molecular dynamics study of the evolution from the formation of the C_6F_6–$(H_2O)_n$ small aggregates to the C_6F_6 solvation

M. Albertí, A. Amat, A. Aguilar, F. Huarte-Larrañaga, J.M. Lucas, F. Pirani and A. Aguilar.

Theor. Chem. Acc., *134* (2015) 61.



Isosurface (isovalue 0.5) plot of the H_2O probability density in the C_6F_6-$(H_2O)_9$ (left-hand side) and the C_6F_6-$(H_2O)_{18}$ (right-hand side) aggregates. Results correspond to Molecular Dynamics simulations at a temperature of 20 K

In this study, the evolution from the formation of small clusters to the solvation of hexafluorobenzene is investigated by means of Molecular Dynamics simulations. For this purpose, the non permanent charge interaction contributions are described using an Improved Lennard-Jones model (ILJ) in combination with the electrostatic energy calculated in agreement with the permanent electric quadrupole and dipole moments of C_6F_6 and H_2O, respectively. To test the potential energy function, three different approaches of H_2O-C_6F_6 have been considered and BSSE-corrected energies at the CCSD(T)/aug-cc-pVTZ level have been calculated for the three approaches. By using the constructed force field, the structure and energetics of some small aggregates, C_6F_6-$(H_2O)_n$ (n = 1–6), the formation of the first solvation shell C_6F_6-$(H_2O)_n$ (n = 9–36) and the solvation of C_6F_6 by 400 molecules of H_2O have been investigated. The small aggregates and the formation of the first solvation shell have been simulated using a microcanonical (NVE) ensemble of particles, while an isobaric–isothermal ensemble (NpT) has been used to investigate the solvation of of C_6F_6. In order to approximate the system formed by one C_6F_6 molecule and 400 H_2O molecules to a large (infinite) system, periodic boundary conditions have been imposed in the simulation of the solvation C_6F_6. It has been found that the first solvation shell is only closed when the number of water molecules exceeds those needed to complete it. This fact evidences a high competition between C_6F_6-H_2O and H_2O-H_2O interactions.

III.2 PUBLICATION LIST

ARTICLES

1. *Theoretical study of the free energy surface and kinetics of the hepatitis C virus NS3/NS4A serine protease reaction with the NS5A/5B substrate. Does the generally accepted tetrahedral intermediate exist?*
J. A. Martínez-González, M. González, L. Masgrau, R. Martínez
ACS Catal. *5* (2015) 246.

2. *A single glycosidase harnesses different pyranoside ring transition state conformations for hydrolysis of mannosides and glucosides.*
A. Tankrathok, J. Iglesias-Fernández, R. J. Williams, S. Pengthaisong, S. Baiya, Z. Hakki, R. C. Robinson, M. Hrmova, C. Rovira, S. J. Williams, J. R. Ketudat Cairns.
ACS Catal. *5* (2015) 6041.

3. *Structural Analysis of the Coordination of Dinitrogen to Transition Metal Complexes*
B. Peigné, G. Aullón.
Acta Cryst., Sect. B *71* (2015) 369.

4. *Assessment of Functionals for First-Principle Studies of the Structural and Electronic Properties of δ-Bi_2O_3.*
D. H. Galván, R. Núñez-González, R. Rangel, P. Alemany, A. Posada-Amarillas
Adv. Cond. Matter Phys. (2015), 120294.

5. *Tuning Crystal Ordering, Electronic Structure, and Morphology in Organic Semiconductors: Tetrathiafulvalenes as a Model Case*
R. Pfattner, S. T. Bromley, C. Rovira, and M. Mas-Torrent.
Adv. Funct. Mat. Accepted. DOI:10.1002/adfm.201502446.

6. *Evidence for a boat conformation at the transition state of GH76 α-1,6-mannanases; key enzymes in bacterial and fungal mannoprotein metabolism.*
A. J. Thompson, G. Speciale, J. Iglesias-Fernández, Z. Hakki, T. Belz, A. Cartmell, R. J. Spears, E. Chandler, J. Stepper, H. J. Gilbert, C. Rovira, S. J. Williams, G. J. Davies.
Angew. Chem. Int. Ed. *54* (2015) 5378.

7. *Ruthenium-catalyzed O- to S-alkyl migration: A pseudoreversible Barton-McCombie pathway.*
W. Mahy, P. Plucinski, J. Jover, C. G. Frost.
Angew. Chem. Int. Ed. *54* (2015) 10944.

8. *Force-induced Reversal of β-Eliminations: Stressed Disulfide Bonds in Alkaline Solution.*
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A.Vilà, M. González, R. Mayol
Phys. Chem. Chem. Phys. *17* (2015) 32241.

108. *Quantum dynamics of the pick up process of atoms by superfluid helium nanodroplets. The Ne + $(^4He)_{1000}$ system.*
A. Vilà, M. González, R. Mayol
Phys. Chem. Chem. Phys. in press (DOI: 10.1039/C5CP04176G).

109. *Relaxation dynamics of helium nanodroplets after photodissociation of a dopant homonuclear diatomic molecule. The case of $Cl_2@(^4He)_N$.*
A. Vilà, M. González, R. Mayol
Phys. Chem. Chem. Phys. in press (DOI: 10.1039/C5CP02679B).

110. *Equilibrium microphase separation in the two-leaflet model of lipid membranes.*
R. Reigada, A. S. Mikhailov.
Phys. Rev. E *(accepted)*.

111. *Nanomechanics of Bidentate Thiolate Ligands on Gold Surfaces*
M. E. Zoloff-Michoff, J. Ribas-Arino, D. Marx
Phys. Rev. Lett. 114 (2015) 075501.

112. *Nickel(II) Complexes having Different Configurations controlled by N,N,O-donor Schiff-base Ligands in Presence of Isothiocyanate as Co-ligand: Synthesis, Structures, Comparative Biological Activity and DFT Study.*
J. Adhikary, P. Kundu, S. Dasgupta, S. Mukherjee, S. Chattopadhyay, G. Aullón, D. Das.
Polyhedron *101* (2015) 93.

113. *Binding of azole drugs to heme: A combined MS/MS and computational approach.*
A. De Petris, M. E. Crestoni, A. Pirolli, C. Rovira, J. Iglesias-Fernández, B. Chiavarino, R. Ragno, S. Fornarini.
Polyhedron *90* (2015) 245.

114. *Methane Capture at Room Temperature: Adsorption on Cubic delta-MoC and Orthorhombic beta-Mo_2C Molybdenum Carbide (001) Surfaces.*
S. Posada-Pérez, J.R.D.S. Politi, F. Viñes, F. Illas.
RSC Adv. *5* (2015) 33737.

115. *Structural control over spin localization in triarylmethyls*
I. Alcon, S. T. Bromley
RSC Adv. *5* (2015) 98593.

116. *Intriguing Electrostatic Potential of CO: Negative Bond-Ends and Positive Bond-Cylindrical Surface.*
H. Kim, V.D. Doan, W.J. Cho, R. Valero, Z. Aliakbar Tehrani, J.M.L. Jenica, K.S. Kim.
Sci. Rep. *5* (2015) 16307.

117. *Design of a Structural Database for Homoleptic Transition Metal Complexes*
J. Fernández-Valparís, S. Alvarez.
Struct. Chem. *26* (2015) 1715.

118. *Surfaces are Different: A Perspective on Structural, Energetic, and Electronic Properties of (001) Surfaces of Alkaline Earth Metal Oxides as Calculated with Hybrid Density Functional Theory.*
Andrew J. Logsdail, David Mora-Fonz, David O. Scanlon, C. Richard A. Catlow, Alexey A. Sokol.
Surf. Sci. *642* (2015) 66.

119. *Exploring the Activity of a Novel Au/TiC(001) Model Catalyst towards CO and CO_2 Hydrogenation.*
G.G. Asara, J.M Ricart, J.A. Rodriguez, F. Illas.
Surf. Sci. *640* (2015) 141.

120. *On the Hydrogen Adsorption and Dissociation on Cu Surfaces and Nanorows.*
L. Álvarez-Falcón, F. Viñes, A. Notario-Estévez, F. Illas.
Surf. Sci. (2015) Accepted.

121. *One-pot synthesis of 4-aminated pyrrolo[2,3-d]pyrimidines from alkynylpyrimidines under metal-catalyst-free conditions.*
V. Prieur, N. Heindler J. Rubio-Martínez ,G. Guillaumet, M. Dolors Pujol.
Tetrahedron 71 (2015) 1207.

122. *Triplet-Singlet Gap in Structurally Flexible Organic Diradicals.*
D.R. Mañeru, I.P.R. Moreira, F. Illas.
Theor. Chem. Acc. *134* (2015) 18.

123. *A molecular dynamics study of the evolution from the fromation of the C_6H_6-$(H_2O)_n$ small aggregates to the C_6F_6 solvation*
M. Albertí, A. Amat, A. Aguilar, F. Huarte-Larrañaga, J.M. Lucas and F. Pirani
Theor. Chem. Acc. *134* (2015) 61.

124. *The Variational Nature of the Gentlest Ascent Dynamics and the Relation of a Variational Minimum of a Curve and the Minimum Energy Path.*
J. M. Bofill, W. Quapp.
Theor. Chem. Acc. (2015) *(accepted)***.**

125. *Fundamentals of Methanol Synthesis on Metal Carbide Based Catalysts: Activation of CO_2 and H_2.*
S. Posada-Pérez, F. Viñes, J.A. Rodriguez, F. Illas.
Top. Catal. 58 (2015) 159.

BOOK CHAPTERS AND PROCEEDINGS

1. *QM/MM calculations on selectivity in homogeneous catalysis*
   J. Jover, F. Maseras.
   Structure and Bonding, in press (2015), doi: 10.1007/430_2015_188

2. Comparison of the Cr-Cr quadruple and quintuple bonding mechanisms
   A. Falceto, S. Alvarez.
   Structure and Bonding, in press (2015), doi: 10.1007/430_2015_191

3. *Ab Initio Wavefunction Approaches to Spin States*
   C. Sousa, C. de Graaf.
   Spin States in Biochemistry and Inorganic Chemistry: Influence on Structure and Reactivity (Wiley)

III.3 OTHER ACTIVITIES

DOCTORALS THESES 2015

1. *A Study of Nanostructuring Effects on Model Heterogeneous Catalysts*
   Sergey M. Kozlov
   Facultat de Química, Universitat de Barcelona
   January 2015

2. *Ab initio molecular dynamics study of thiolate-protected gold clusters and their interaction with biomolecules.*
   Víctor Rojas Cervellera
   Universitat Politècnica de Catalunya.
   July 2015

3. *Quantum dynamics of physicochemical processes in superfluid ^{4}He nanodroplets.*
   Arnau Vilà Casanovas
   Facultat de Química, Universitat de Barcelona
   September 2015

4. *Radical-pair formation in organic π-stacked architectures*
   Maria Fumanal Quintana
   Facultat de Química, Universitat de Barcelona
   October 2015

MASTERS THESES 2015

1. *Structure, elastic and electronic properties of pristine and doped graphyne. A DFT study.*
   Antonio Ruiz Puigdollers
   Facultat de Química, Universitat de Barcelona
   July 2015

2. *Theoretical study of the adsorption of N_2, O_2 and CO_2 in different faujasite structures.*
   Gerard Alonso Benito
   Facultat de Química, Universitat de Barcelona
   July 2015

3. *Kinetic Monte Carlo simulations of the water-gas shift reaction on copper catalysts from density functional theory based calculations*
Hèctor Prats Garcia
Facultat de Química, Universitat de Barcelona
July 2015

4. *Optimització d'un camp de forces reactiu per l'adsorció de CO_2 sobre X-zeolita (X=Ca, Na).*
Núria Sambola Marcial
Facultat de Química, Universitat de Barcelona
July 2015

5. *Angular momentum effects on the pick up process of neon atoms by superfluid helium nanodroplets.*
Miquel Blancafort Jorquera
Facultat de Química, Universitat de Barcelona.
July 2015

6. *Crowding Effects on Oligomeric Enzymes: Kinetics Analysis of the ALKP-Catalyzed Hydrolysis*
Claudia Hernández Carro
Facultat de Farmàcia, Universitat de Barcelona.
July 2015

7. *Capture of Ne atoms by ^{4}He nanodroplets at low energies. Quantum vs. classical comparison at J=0.*
Arturo Sopena Moros
Facultat de Química, Universitat de Barcelona.
July 2015

8. *Simulació de l'adsorció de gasos en metal- organic frameworks, usant un camp de forces reactiu.*
Carles Martí Aliod
Facultat de Química, Universitat de Barcelona.
July 2015

SCIENTIFIC CONFERENCES AND MEETINGS 2015

Journées de la Division Chimie de Coordination (JCC) de la Société Chimique de France
Talence (France)

Analyse de forme des composées de coordination (plenary lecture).
S. Alvarez.

ACS National Meeting
Boston (USA)

Reaction pathway prediction and differentiation in the TBP geometries found in vanadium-phoshpatase protein complexes using shape analysis.
I. Sánchez-Lombardo, S. Alvarez, C. McLauchlan, D. C. Crans.

Computational modeling of nanostructured ceria for the rational design of catalytic materials
A. Bruix, A. Figueroba, F. Illas, K.M. Neyman

Pacifichem 2015,
Honolulu (USA)

Distortions in decavanadates and how that may impact interactions with biological interfaces. (comunicació oral).
D. C. Crans, I. Sánchez-Lombardo, S. Alvarez, N. Levinger.

European Workshop on Theoretical approaches of Molecular Magnetism: Jujols VIII
Bages (France)

Spin Crossover-induced Changes in the Coordination Sphere.
S. Alvarez.

Room temperature magnetoresistance in single-molecule devices.
E. Ruiz.

Modeling the ligand tuning effect over the transition temperature in Spin-Crossover systems using Density Functional Methods.
J. Cirera.

Workshop aportando valor al CO_2, organized by The Spanish Technological Platform for CO_2 (PTECO2) and the Spanish Technological Platform for Sustainable Chemistry (SusChem)
Madrid (Spain)

Influence of impurities in CO_2 capture over a zeolitic material
A. Díaz-Márquez, P. Gamallo, D. Bahamón, L. F. Vega

6th Iberian Meeting on Colloids and Interfaces (RICI6)
Gimerães (Portugal)

CO_2 separation from multicomponent mixtures by adsorption in MOF Cu-BTC and zeolite 13X
D. Bahamon, A. Diaz-Marquez, P. Gamallo, L. F. Vega

In-vivo-like study of the excluded volume effects on the kinetics of enzymatic reactions
C. Balcells, C. Hernández, M. Via, I. Pastor, C. Rey-Castro, J.L. Garcés, S. Madurga, E. Vilaseca, M. Cascante, F. Mas

Crowding effects on oligomeric enzymes: kinetic analysis of the ALKP-catalyzed hydrolysis
C. Hernández, C. Balcells, M. Via, I. Pastor, J.L. Garcés, S. Madurga, M. Cascante, F. Mas

Dissolution of nanomaterals in the context of safety assessment studies. Relevance of dynamic and equilibrium speciation techniques
C. Rey-Castro, C.A. David, S. Cruz-González, J. Salvador, F. Mas, J. Galceran, J. Puy

Coupling of conformational and ionization equilibria in a linear polymer. The site binding/rotational state (SBRIS) modelling
S. Madurga, J.L. Garcés, M. Borkovec

Masterquímica XI
Barcelona (Spain)

Estudi teòric de l'adsorció de O_2, N_2 i CO_2 sobre faujasites amb diferents distribucions de Na+ preadsorbit
G. Alonso, R. Sayós, X. Giménez, P. Gamallo

Efecte de l'aglomeració macromolecular en enzims oligomèrics; anàlisi cinètica de la hidròlisi de fosfat catalitzada per ALKP
C. Hernández, C. Balcells, M. Via, I. Pastor, J.L. Garcés, S. Madurga, M. Cascante, F. Mas

Simulació per Dinàmica Browniana de processos de reacció-difusió de proteïnes en medis intracel·lulars
M. Via, P.M. Blanco, S. Madurga, E. Vilaseca, F. Mas

XXXI Annual meeting of the reference network of R+D+I on Theoretical and Computational Chemistry
Girona (Spain)

Effect of Na^+ addition of O_2, N_2 and CO_2 on Faujasite frameworks: a DFT study
G. Alonso, R. Sayós, X. Giménez, L. F. Vega, P. Gamallo

Effects of reaction conditions on copper-catalyzed water-gas shift reaction: a kinetic Monte Carlo study
H. Prats, L. Álvarez, F. Illas, R. Sayós

Ionization mechanism of citric acid in water. An ab initio study and statistical-mechanics treatment of NMR titration data.
S. Madurga, J.L. Garcés, M. Nedyalkova, F. Mas

Fundamentals of Methanol Synthesis on Molybdenum Carbide Based Catalysts
S. Posada-Pérez, F. Viñes, P.J. Ramírez, J.A. Rodríguez, F. Illas

Magnetic Coupling in Heterodinuclear Complexes
D. Reta-Mañeru, R. Costa, R. Valero, I.P.R. Moreira, F. Illas

Triarylmethyl Radicals: Tunneable Building Blocks for Molecular Spintronics
I. Alcón, S.T. Bromley

Effects of Reaction Conditions on Copper-Catalyzed Water-Gas-Shift Reaction: A Kinetic Monte Carlo Study
H. Prats, L. Álvarez-Falcón, F. Illas, R. Sayós

VI IQTCUB Symposium
Barcelona (Spain)

Theoretical study of O_2, N_2 and CO_2 adsorption over faujasites with different preadsorbed Na^+ distributions
G. Alonso, R. Sayós, X. Giménez, L. F. Vega, P. Gamallo

Crowding effects on oligomeric enzymes: kinetic analysis of the ALKP-catalyzed hydrolysis
C. Hernández, C. Balcells, M. Via, I. Pastor, J.L. Garcés, S. Madurga, M. Cascante, F. Mas

Brownian motion simulations of reaction-diffusion processes of proteins in intraacellular media
P.M. Blanco, M. Via, S. Madurga, J.L. Garcés, E. Vilaseca, F. Mas

Coupling of conformational and ionization equilibria in a linear polymer. The site binding/rotational state (SBRIS) modelling
S. Madurga, J.L. Garcés, M. Borkovec

Stabilization of Open-Shell States in Purely Organic Molecules
D. Reta

Effects of Reaction Conditions on Copper-Catalyzed Water-Gas-Shift Reaction: A Kinetic Monte Carlo Study
H. Prats, L. Álvarez-Falcón, F. Illas, R. Sayós

Accurate determination of chemical ordering in several nm large bimetallic nanoparticles
G. Kovács, S. M. Kozlov, R. Ferrando, K. M. Neyman

10th European Conference on Computational Chemistry
Fulda (Germany)

Water gas shift reaction on Cu(111) surface: A first-principles based kinetic Monte Carlo study
R. Sayós, H. Prats, L. Álvarez, F. Illas

QM/MM study of a viral serine protease reaction mechanism: Importance of the active centre description
J. A. Martínez, M. González, A. Skelton

European Conference on Surface Science (ECOSS 31)
Barcelona (Spain)

DFT study of the Si/Al ratio in the adsorption of O_2, N_2 and CO_2 on faujasite.
G. Alonso, R. Sayós, X. Giménez, L. F. Vega, P. Gamallo

Influence of step sites in the water-gas shift reaction on copper surfaces
H. Prats, L. Alvarez, P. Gamallo, F. Illas, R. Sayós

IV New trends in Computational Chemistry for Industry Applications
Barcelona (Spain)

Impact of van der Waals interactions on the water gas shift reaction over copper surfaces
H. Prats, L. Álvarez, P. Gamallo, F. Illas, R. Sayós

The importance of framework cations in the selective adsorption of CO_2 compared to O_2 and N_2 in faujasite structures.
G. Alonso, R. Sayós, X. Giménez, P. Gamallo

In-vivo-like study of the excluded volume effects on the kinetics of enzymatic reactions
C. Balcells, C. Hernández, M. Via, I. Pastor, C. Rey-Castro, J.L. Garcés, S. Madurga, E. Vilaseca, M. Cascante, F. Mas

Brownian motion simulations of reaction-diffusion processes of proteins in intraacellular media
P.M. Blanco, M. Via, S. Madurga, J.L. Garcés, E. Vilaseca, F. Mas

Triarylmethyl Radicals: Potential Building Blocks for Molecular Spintronics
I. Alcón, D. Reta, I.P.R. Moreira, S.T. Bromley

Impact of van der Waals Interactions on the Water Gas Shift Reaction over Copper Surfaces
H. Prats, L. Álvarez-Falcón, P. Gamallo, F. Illas, R. Sayós

Surface Contact Engineering in Photoactive ZnO Nanostructures
O. Lamiel-García, F. Viñes, A. Iglesias-Juez, M. Fernández-García, F. Illas

Electronic-Structure-Based Chemical Descriptors: (In)Dependence on Self-Iteraction and Hartree-Fock Exchange
A. Notario-Estévez, S.M. Kozlov, F. Viñes, F. Illas

Performance of Density Functional Theory Based Methods in Predicting Core-Level Binding Energies and the Physical Meaning of Kohn-Sham Orbital Energies
N. Pueyo-Bellafont, P.S. Bagus, F. Illas

Effect of charge transfer between CeO_2(111) support and Pt nanoparticles on their properties
S.M. Kozlov, K.M. Neyman

Accurate determination of chemical ordering in several nm large bimetallic nanoparticles
G. Kovács, S. M. Kozlov, R. Ferrando, K. M. Neyman

First approach to the diffusion of hydrogen confined in single-walled carbon nanotubes using 6D quantum dynamics
M. Mondelo-Martell, F. Huarte-Larrañaga

4th workshop on Theoretical Chemistry and Computational Modeling
Madrid (Spain)

Studying the CO_2 capture problem in dry air through DFT calculations applied of faujasite frameworks
G. Alonso, R. Sayós, X. Giménez, P. Gamallo

Kinetic Monte Carlo simulations of the water-gas shift reaction on copper catalysts from DFT calculations.
H. Prats, L. Álvarez. P. Gamallo, F. Ilas, R. Sayós

XV Congress of the Spanish Biophysical Society (SBE 2015)
Granada (Spain)

In-vivo-like study of the excluded volume effects on the kinetics of enzymatic reactions
C. Balcells, C. Hernández, M. Via, I. Pastor, J.L. Garcés, S. Madurga, E. Vilaseca, M. Cascante, F. Mas

Brownian motion simulations of reaction-diffusion processes of proteins in intraacellular media
M. Via, P.M. Blanco, S. Madurga, J.L. Garcés, E. Vilaseca, F. Mas

Crowding effects on oligomeric enzymes: kinetic analysis of the ALKP-catalyzed hydrolysis
C. Hernández, C. Balcells, M. Via, I. Pastor, J.L. Garcés, S. Madurga, M. Cascante, F. Mas

Congress of Theoretical Chemists of Latin Expression – Chitel 2015
Torino (Italy)

Performance of Exchange-Correlation Functionals on Transition Metals
F. Viñes

Computational Approaches to Materials Design – CAMD 2105
Aveiro (Portugal)

Performance of Exchange-Correlation Functionals on Transition Metals
F. Viñes

Sociedad Española de Catálisis – SECAT 2015
Barcelona (Spain)

Catalizadores de Carburo de Molibdeno para la Síntesis de MEtanol
S. Posada-Pérez, F. Viñes, J.A. Rodríguez, F. Illas

9th RES Users' Conference & 4th Annual HPC Advisory Council Spain Conference
Barcelona (Espanya)

Supercomputation and Realistic Models of Photocatalysts Nanoparticles
F. Illas

CECAM workshop: Emergent structural and electronic phenomena at interfaces of nanoscale oxides
EPFL, Lausanne (Switzerland)

A plethora of polymorphs: oxide nanofilms and nanoporous oxide phases from structure prediction
S.T. Bromley
Nanostructured metal oxides and transition metal nanoparticles interacting with oxide surfaces from density-functional modelling
S.M. Kozlov, K.M. Neyman

ELECSPIN 2015 – International Workshop on Organic and Graphene ELECtronics and SPINtronics
UAB centro de congreses, Barcelona (Spain)

Controlling Spin Localisation in Tryarylmethyl Radicals
S. T. Bromley

FOXES (Formation of Oxides around Evolved Stars) kick-off meeting
Bildungszentrum Hotel, Basel (Switzerland)

Structures of Oxide Clusters Entering Dust Formation
S. T. Bromley

Gordon Research Conference: Clusters & Nanostructures
Melia Golf Vichy Catalan Business and Convention Center, Girona (Spain)

Metal Oxides and their Alloys: Clusters versus Bulk
S. T. Bromley

British Association for Crystal Growth 46th Annual Conference
Queen Mary University of London, London (United Kingdom)
Nanocrystals versus nanoclusters: limits on crystallinity and small size
S. T. Bromley

Workshop: Silicates in Space 2015
University of Heidelberg, Heidelberg (Germany)

Nucleation of SiO and Silicates from the Bottom-up
S. T. Bromley

Workshop "Catalysis Meets Sensing"
Karlsruhe Institute of Technology, Karlsruhe (Germany)

Density-functional modelling of metal-metaloxide nanostructures for catalysis and energy technologies
K.M. Neyman

International FOXSI Symposium, SFB "Functional Oxide Surfaces and Interfaces (FOXSI)" (May 11-13, invited lecture)
Institute of Materials Chemistry, Vienna University of Technology, Vienna (Austria)

Metal-metaloxide nanostructures in catalysis and energy technologies from a viewpoint of density functional modelling
K.M. Neyman

International Symposium on Frontiers in Computational Catalysis
Tsinghua University, Beijing (P.R. China)

Theoretical modelling in heterogeneous catalysis: As simple as possible, but not simpler
K.M. Neyman

11th International Conference on Diffusion in Solids and Liquids
Munich (Germany)

Interactions of hydrogen with transition metal nanoparticles from first principles
K.M. Neyman

CECAM Workshop "Modeling metal-based nanoparticles: toward realistic environments"
CEMES, Tolouse (France)

As simple as possible, but not simpler: Density-functional modelling of metal nanoparticles in catalysis
K.M. Neyman

XII European Congress on Catalysis (EuropaCat) "Catalysis: Balancing the use of fossil and renewable resources" (August 30-September 4, keynote lecture)
Kazan (Russia)

Approaching complexity in heterogeneous catalysis by density-functional modelling
K.M. Neyman

A GGA+U DFT investigation of silver atom, trimer and tetramer supported by a nanosized particle $Ce_{21}O_{42}$
V.A. Nasluzov, S. Laletina, E.I. Ivanova Shor, A.M. Shor, K.M. Neyman

Thomas Young Centre, The London Centre for the theory and Simulation of Materials
London (United Kingdom)

As simple as possible, but not simpler: DFT modelling of nanostructures in catalysis and energy technologies
K.M. Neyman

Chemical Reactions at Surfaces (Gordon Research Seminar), Surface Science Techniques for Addressing Contemporary Issues
Ventura (USA)

Combining theory and experiment for the rational design of nanostructured Pt-CeO_2 catalytic materials with maximum noble-metal efficiency
A. Bruix, A. Figueroba, Y. Lykhach, I. Matolínová, A. Neitzel, T. Skála, N. Tsud, M. Vorokhta, V. Stetsovych, K. Ševčiková, J. Mysliveček, K.C. Prince, F. Illas, V. Matolín, J. Libuda, K.M. Neyman

3S15 28th Symposium on Surface Science (3S15)
Les Arcs 1800 (France)

Atomically dispersed and oxide-supported platinum in fuel cell catalysis: from surface science to in-situ spectroelectrochemistry
J. Libuda, O. Brummel, A. Bruix, Y. Lykhach, I. Matolínová, A. Neitzel, F. Faisal, T. Skála, N. Tsud, M. Vorokhta, V. Stetsovych, K. Ševčiková, J. Mysliveček, I. Khalakhan, R. Fiala, M. Václavů, K.C. Prince, F. Illas, V. Matolín, K.M. Neyman

International Workshop "Low-precious-metal-content catalysts for PEM fuel cells"
Dijon (France)

Computational studies of nanoparticulate models of catalysts in the ChipCAT project
K.M. Neyman

Tuning Pt catalysts for fuel cells by metal-oxide interactions
S.M. Kozlov, K.M. Neyman

Modeling interactions of transition metal species with ceria nanoparticles for applications in fuel cell catalysts
A. Figueroba, G. Kovács, A. Bruix, K.M. Neyman

Surface composition of magnetron sputtered Pt-Co thin film catalyst for proton exchange membrane fuel cells
M. Vorokhta, M. Václavů, I. Khalakhan, R. Fiala, P. Kúš, T. Skála, N. Tsud, J. Lavková, V. Potin, I. Matolínová, G. Kovács, S.M. Kozlov, K.M. Neyman, V. Matolín

WG3 Meeting of the COST Action CM1104 "Reducible oxide chemistry, structure and functions"
Poznan (Poland)

Recent progress in density functional studies of ceria-based nanostructures: Inspiration by experimentalists from Erlangen and Prague
A. Figueroba, S.M. Kozlov, K.M. Neyman

XXVI International Symposium on Molecular Beams (ISMB 2015)
Parador of Segovia, Segovia (Spain)

Dynamics and kinetics of the $X + H_2^+ \rightarrow XH_2^+$ (X=He, Ne, Ar) capture processes as a function of temperature
P. A. Enríquez, M. P. Puyuelo, R. Martínez, P. Gamallo, M. González

Dynamics and kinetics of $O + H_2^+ \rightarrow OH^+ + H$, $OH + H^+$ on the two lowest potential energy surfaces
R. Martínez, M. Paniagua, C. Petrongolo, P. Gamallo, J. Mayneris-Perxachs, M. González

Stereodynamics and reaction mode of the $O(^3P) + CH_4, CD_4 \rightarrow OH + CH_3, OD + CD_3$ combustion reactions on the ground PES
R. Martínez, P. A. Enríquez, M. P. Puyuelo, M. González

Guided ion beam and ab initio studies of the $Na^+ + i\text{-}C_3H_7Br$ and $Na^+ + i\text{-}C_3H_7OH$ gas phase reactive collisions
E. López, J. M. Lucas, J. de Andrés, M. Albertí, J. M. Bofill, D. Basi, A. Aguilar.

Ion-molecule collisions: Crossed-beams and guided-ion-beams and computational studies of reactive processes
E. López, J.M. Lucas, J. De Andrés, M. Albertí and A. Aguilar

Quantum Dynamics Study of the H2 molecule confined in Single-walled Carbon Nanotubes
M. Mondelo-Martell, F. Huarte-Larrañaga

XIII International Workshop on Quantum Reactive Scattering (QRS 2015)
University of Salamanca, Salamanca (Spain)

Quantum dynamics of chemical and physical processes involving superfluid helium nanodroplets
A. Vilà, M. González, R. Mayol

Born-Oppenheimer and Renner-Teller coupled-channel quantum reaction dynamics of O + H_2^+ collisions
P. Gamallo, P. Defazio, C. Petrongolo, M. Paniagua, M. González

The 5th Workshop Quantum Days in Bilbao Quantum Days in Bilbao: Mathematical Methods in Atomic and Molecular Physics
BCAM - Basque Center for Applied Mathematics, Bilbao (Spain)

Quantum dynamics of physicochemical processes involving atoms or molecules and superfluid ^{4}He nanodroplets
A. Vilà, M. González, R. Mayol

24th International Symposium on Ion Atom Collisions (ISIAC 2015)
Sant Jordi College, University of Barcelona, Barcelona (Spain)
Symposium organized by members of IQTCUB: A. Aguilar (Chair), M. Albertí, J. de Andrés, J.M. Lucas, F. Huarte (Secretary)

Born-Oppenheimer and Renner-Teller coupled-channel quantum reaction dynamics of O + $H_2^+ \rightarrow OH^+ + H$, $OH + H^+$
M. González, P. Gamallo, P. Defazio, M. Paniagua, C. Petrongolo

An environmentally relevant process: Collisions between ground state Na ions and N_2O molecules in the 0.1-5 KeV
J. de Andrés, J. M. Lucas, A. Aguilar, J. M. Bofill, M. Albertí, E. López.

Experimental and computational study of the Li^+ + i-C_3H_7Br and Li^+ + i-C_3H_7OH gas phase reactive collisions
A. Aguilar, E. López, J. M. Lucas, J. de Andrés, M. Albertí, J. M. Bofill.

Ion-molecule collisions in Titan´s atmosphere: A prebiotic mechanism
E. López, D. Ascenzi, J. M. Bofill, A. Aguilar.

Quantum dynamics of the hydrogen molecule diffusion along a single-walled carbon nanotube
M. Mondelo-Martell, F. Huarte-Larrañaga

Spanish-Italian Medicinal Chemistry Congress (SIMMC 2015),(PRBB)
PRBB, Barcelona (Spain)

Design, Synthesis, cell growth inhibition and antitumor screening of New 6,9-disubstituted Purines by inhibition of CDK4/6
A. Vinuesa, O. Abián, J. Rubio, MD. Pujol.

Design, Synthesis and Biological Activity of new K-ras inhibidors
L. Grau, R. Soucek, J. Rubio, MD. Pujol

II Simposio de Jóvenes Investigadores de la Sociedad Española de Química Terapéutica.
Barcelona (Spain)

Studies of CDK4/6 inhibitors such as antitumor agents: Design, Synthesis and cell growth inhibition
A.Vinuesa, O. Abián, J. Rubio, MD. Pujol

Preparation of new pyrazolidin-3-ones. Evaluation of their antitumor activity by K-ras inhibition
L. Grau, R. Soucek, J. Rubio, MD. Pujol

15-th V.A. Fock Meeting on Quantum and Computational Chemistry
Federal Far East University, Vladivostok (Russia)

Analyzing the Interplay Between Local and Global Symmetries in Molecular Chemistry
P. Alemany

3rd International Conference on Materials Science
Universidad Austral de Chile, Valdivia (Chile)

Continuous Shape and Symmetry Measures: a new Tool for Structural Characterization
P. Alemany

Molecular Quantum Dynamics: Benchmarks and State of the Art
CECAM, Lausanne (Switzerland)

Nonadiabatic Molecular Dynamics with Conditional Wave Functions
G. Albareda, J. M. Bofill, A. Abedi, I. Tavernelli, A. Rubio.

Psi-k 2015 Conference
Kursaal, San Sebastià (Spain)

Adiabatic and Nonadiabatic Molecular Dynamics with Conditional Wave Functions
G. Albareda, J. M. Bofill, A. Abedi, I. Tavernelli, A. Rubio.

International Conference on Unsolved Problems on Noise
Casa de la Convalescència, Barcelona (Spain)

Role of Current-Voltage Correlations on the Electric Power of Nanoscale Devices
G. Albareda, F. L. Traversa, and X. Oriols.

Current Fluctuations Originating from Non-Metallic (Physical) Leads
G. Albareda, L. Chen, X. Oriols, I. Franco.

XXIX International Conference on Photonic, Electronic and Atomic Collisions (ICPEAC 2015)
Toledo (Spain)

Crossed-beams and ab initio study of the gas phase charge transfer with excitation in N_2O and Li^+ collisions of environmental interest
J. de Andrés, J. M. Lucas, M. Albertí, J. M. Bofill, A. Aguilar.

Quantum dynamics of the hydrogen molecule confined in single-walled carbon nanotubes
M. Mondelo-Martell, F. Huarte-Larrañaga

ICIQ-FIFC Spain-Japan Symposium on Theoretical and Computational Chemistry of Complex Systems
Tarragona (Spain)

Exploring Potential Energy Surfaces of Complex Molecular Systems using Zermelo's Navigation Variational Model
J. M. Bofill, W. Quapp, I. de P. R. Moreira.

How Does Nature Make Glycosidic Bonds. Ab initio QM/MM Metadynamics Investigations
C. Rovira

CECAM School: Quantum dynamics in molecular systems: theory, modelling, simulation.
IDRIS (Institut du développement des ressources informatiques et scientifiques), Orsay (France)

Diffusion of hydrogen along SWCNT: a first approach using quantum dynamics methods
M. Mondelo-Martell, F. Huarte-Larrañaga

2nd BSC International Doctoral Symposium
Universitat Politècnica de Catalunya, Barcelona (Spain)

Quantum dynamics study of the hydrogen molecule confined in single-walled carbon nanotubes
M. Mondelo-Martell, F. Huarte-Larrañaga

Virtual Environments and detailed simulations of molecular processes, Symposium in honor of Prof. A. Laganà
MonteLino, Bettona, Perugia (Italy)

Experimental and computational studies of ion-molecule reactions
A. Aguilar

Explicit control over spin states in technology and biochemistry (ECOSTBIO) workshop
University of Marseille, Marseille (França)

An ionizable triptophan residue imparts catalase activity to a peroxidase core. Insights from QM/MM simulations
C. Rovira

Carbohydrate active enzymes in medicine and biotechnology
University of St. Andrews, St. Andrews (UK)

Sugar conformational changes and reactivity of carbohydrate-active enzymes. Ab initio QM/MM metadynamics investigations
C. Rovira

Future trends in protein science. 13th workshop in Protein.DTU
Technical University of Denmark, Lyngby (Denmark)

How Does Nature Make Glycosidic Bonds
C. Rovira

Glycosyl cation day
University of Poitiers, Poitiers (France)

Sugar conformational changes and reactivity of carbohydrate-active enzymes. Ab initio QM/MM metadynamics investigations
C. Rovira

RESEARCH STAYS IN RECOGNIZED CENTERS

P. Gamallo **MATGAS, Barcelona (Spain)**
Invited visiting professor. January-February 2015

G. Alonso **MATGAS, Barcelona (Spain)**
Invited visiting professor. January-June 2015

M. Albertí **Univeristà di Perugia, Perugia (Italy)**
Research stay. February-July 2015

M. Mondelo Martell **University of Bielefeld, Bielefeld (Germany)**
Predoctoral stay. March-April 2015

J. Jornet Somoza **University of the Basque Country, San Sebastián (Spain)**
Research stay. April-July 2015

R. Reigada **Max Planck Institute, Berlin (Germany)**
Invited visiting professor. May 2015

G. Albareda **Max Planck for the Structure and Dynamics of Matter**, **Hamburg (Germany)**
Invited visiting scientist. July 2015

J. Ribas **University of Wroclaw, Wroclaw (Poland)**
Invited visiting scientist. July 2015

K.M. Neyman **Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen (Germany)**
Invited visiting scientist. July-August 2015

C. Climent **Donostia International Physics Center, Donostia (Spain)**
Predoctoral research stay. July and September 2015

P. Alemany **Departamento de Química, Universidad Católica del Norte, Antofagasta (Chile)**

Invited visiting scientist. October 2015

S. Posada-Pérez **Brookhaven National Laboratory, Upton (USA)**

Predoctoral stay. October-December 2015

PARTICIPATION IN COMPETITIVE FUNDED RESEARCH PROJECTS

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

Grup d'Estructura Electrònica.
Santiago Alvarez Reverter, Universitat de Barcelona
2014SGR662, 2014-2016
Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR)

Grup de Bioquímica Integrativa
Marta Cascante Serratosa, Universitat de Barcelona
2014SGR1017, 2014-2016
Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR)

Simulació molecular aplicada (MOLSIMAP)
Lourdes Vega Fernández, MATGAS
2014SGR1582, 2014-2016
Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR)

Grup de Recerca Reconegut i Finançat per la Generalitat de Catalunya
Francesc Illas Riera
Universitat de Barcelona
2014SGR97, 2014-2016
Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR), Generalitat de Catalunya

Grup de Dinàmica de Reaccions Químiques
Antonio Aguilar Navarro, Universitat de Barcelona
2014SGR0025, 2014-2016
Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR)

Química Orgànica Experimental, Teòrica i Computacional
Josep Maria Bofill Vilà, Universitat de Barcelona
2014SGR139, 2014-2016
Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR)

Estructura i funció en macromolècules
Carme Rovira Virgili, Universitat de Barcelona
2014SGR-987, 2014-2016
Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR)

ICREA Acadèmia
Eliseo Ruiz, Universitat de Barcelona
2014-2018,
ICREA (Generalitat de Catalunya)

Simulación de sistemas cuánticos nanostructurados fuera equilibrio.
Angel Rubio Secades, Universitat del País Basc
IT578-13, 2013-2018
Comunidad Autónoma del País Basco

Estructura electrónica y propiedades de moléculas y sólidos inorgánicos.
Eliseo Ruiz Sabín, Universitat de Barcelona
CTQ2011-23862-C02, 2012-2014, extended until 6/2015.
MICINN

Mecanismo de transición de fase e interacción magnética en cristales moleculares magnéticos que presentan transición de espín
Juan J. Novoa Vide and Mercè Deumal, Universitat de Barcelona
MAT2014-54025-P, 2015-2017
Ministerio de Economia y Competitividad (MINECO)

Captura y separación de gases y contaminantes en procesos Industriales sostenibles
Ramón Sayós Ortega / Pablo Gamallo Belmonte, Universitat de Barcelona
CTQ2014-53987-R, 2015-2017
Ministerio de Economia y Competitividad (MINECO)

Fisicoquímica de las interacciones y fenómenos de transporte a nivel coloidal entre iones, macromoléculas y nanopartículas de interés ambiental
Francesc Mas Pujadas, Universitat de Barcelona
CTM2012-39183-C02-02, 2013-2015
Ministerio de Economia y Competitividad (MINECO)

Quantum-chemical study and computational design of advanced materials
Francesc Illas Riera, Universitat de Barcelona
CTQ2012-30751, 2013-2015
Ministerio de Economia y Competitividad (MINECO)

Modelizacion de Materiales Formados por Mezclas de Oxidos con Relavancia Tecnologica y Medioambiental.
Stefan Bromley, Universitat de Barcelona
MAT2012-30924, 2012-2015
Ministerio de Economia y Competitividad (MINECO)

Theoretical modeling of the reactivity of nanostructures relevant to catalysis and to energy technologies
Konstantin Neyman, Universitat de Barcelona
CTQ2012-34969, 2013-2015
Ministerio de Economía y Competitividad (MINECO)

Estudio teórico de la dinámica y cinética de reacciones químicas. Química atmosférica, procesos de combustión y aplicaciones a sistemas enzimáticos.
Miguel González Pérez, Universitat de Barcelona
CTQ2011-27857-C02-01, 2012-2015
Dirección General de Investigación (DGI)

Dispositivos Electrónicos de baja Dimensionalidad para Aplicaciones de Radiofrecuencia y Digitales: Simulación y Desarrollo de Software.
Xavier Oriols Pladevall, Universitat Autònoma de Barcelona
TEC2012-31330, 2013-2015
Ministerio de Economia y Competitividad (MINECO)

Experimentación y modelización computacional de dinámica de reacciones químicas.
Antonio Aguilar Navarro (IP1), Fermín Huarte Larrañaga (IP2), Universitat de Barcelona
CTQ2013-41307-P, **2014-2016**
Ministerio de Economía y Competitividad (MINECO)

Moduladores fotoconmutables sintéticos para manipular remotamente proteínas endógenas: fotocontrol in vivo de canales iónicos pentaméricos.
Carme Rovira Virgili, Universitat de Barcelona
PCIN-2015-163-C02-01, 2015-2017
Ministerio de Economia y Competitividad (MINECO)

Simulation of reactive processes in proteins and enzymes by means of ab initio molecular dynamics and QM/MM techniques.
Carme Rovira Virgili, Universitat de Barcelona
CTQ2014-55174-P, 2015-2017
Ministerio de Economia y Competitividad (MINECO)

Materia blanda forzada, activa y viva.
Jaume Casademunt Viader and Francesc Sagués Mestre, Universitat de Barcelona
FIS2013-41144P, 2014-2016
Ministerio de Economia y Competitividad (MINECO)

El dominio único de c-Src: dominios proteicos desordenados en la superficie de la membrana celular .
Miquel Pons Vallès, Universitat de Barcelona
BIO2013-45793-R, 2014-2016
Ministerio de Economia y Competitividad (MINECO)

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

Computational modelling and molecular dynamics simulations of oil/water wettability on carbonate rocks and clays
Ramón Sayós Ortega / Pablo Gamallo Belmonte, Universitat de Barcelona
Referència, 308465
Contracto de arrendamientos y servicios de I+D con REPSOL, S.A.

COMPHOTOCAT: - Computational design of TiO_2 based nanoparticles for improved photocatalytic activity towards water splitting under visible sunlight
Francesc Illas Riera
Universitat de Barcelona
PRACE - 2014112608, 2015-2016
Partnership for Advanced Computing in Europe (PRACE)

Reducible oxide chemistry, structure and functions
Francesc Illas Riera, (representative in Spain), Konstantin Neyman (deputy representative in Spain),
Universitat de Barcelona
CM1104, 2012-2016
European Framework for Cooperation in Science and Technology (COST)

Explicit Control Over Spin-States in Technology and Biochemistry
Marcel Swart (University of Girona), Carme Sousa Romero (participant of the Universitat of Barcelona)
Universitat de Barcelona
CM1305, 2014-2018
European Framework for Cooperation in Science and Technology (COST)

Nanostructured materials for solid-state hydrogen storage
Konstantin Neyman, Universitat de Barcelona (member)
MP1103, 2011-2015
European Framework for Cooperation in Science and Technology (COST)

Design of thin-film nanocatalysts for on-chip fuel cell technology
Konstantin Neyman, Universitat de Barcelona
FP7-NMP.2012.1.1-1, Ref. No.310191, 2012-2016
European FP7 'Cooperation' - Research theme: 'Nanosciences, nanotechnologies, materials and new production technologies'

Theoretical Chemistry and Computational Modelling
Juan Novoa Vide, Universitat de Barcelona
H2020-MSCA-ITN-2014-642294
Horizon 2020, Innovative Training Networks

A comprehensive and standardised e-infrastructure for analysing medical metabolic phenotype data (PhenoMeNal)
Marta Cascante Serratosa
8P1MCA - HORIZON 2020, 2015-2018.
European Union.

PhenoMeNal: A comprehensive and standardised e-infrastructure for analysing medical metabolic phenotype data (PhenoMeNal).
Marta Cascante Serratosa, Universitat de Barcelona
654241, 2015-2018
European Union

Deciphering the Metabolism of Haematological Cancers (HaemMetabolome)
Marta Cascante Serratosa, Universitat de Barcelona
675790, 01/10/2015- 30/09/2019
European Union

NOMAD – Novel Materials Discovery
Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin
NoMaD - 676580, 2015-2018
Horizon 2020-EINFRA-5-2015, Centers of Excellence for Computing applications

Device simulation (RF), NannoMechanics and Spintronics.
David Jiménez Jiménez, Universitat Autònoma de Barcelona
604391 Graphene, 2013-2016
European Commission (FET Flagship)

Dynamical processes in open quantum systems: pushing the frontiers of theoretical spectroscopy (DYNAMO).
Angel Rubio Secades, Universitat del País Basc
ERC-2010-AdG_20100224, 2011-2016
European Research Council (ERC)

Institut de Química Teòrica
i Computacional