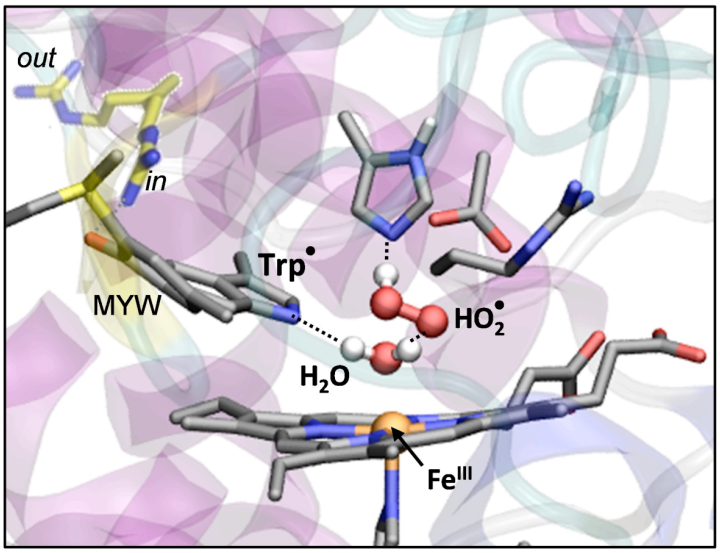
Institut de Química Teòrica i Computacional

UNIVERSITAT DE BARCELONA

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



Activity Report 2014

On November 27th, 2007 the Board of Government of the *Universitat de Barcelona* (UB) approved the creation of the Institute of Theoretical Chemistry of the *Universitat de Barcelona* (IQTCUB), one of the research institutes of this university. IQTCUB brings together professors and researchers from different departments of the Chemistry and Physics faculties of UB who commonly use methods of Computational Chemistry and/or Computational Physics (e.g. Quantum Chemistry, Solid State Modeling). The IQTCUB research activity, if mainly within the field of Chemistry, is quite different from what one expects from a traditional chemist. This is because 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 if not thousands of processors. The main goals of Theoretical and Computational Chemistry are: to reach a detailed knowledge of chemical process at the molecular level, to make predictions which can be experimentally proven, to interpret experimental results, and to create new tools and concepts. From such a basis the IQTCUB aims to design new materials and drug molecules with tailored properties, investigate new chemical reactions to obtain important 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. Obviously, most of these goals are also shared with other scientific disciplines. Precisely because of the interdisciplinary approach of modern research, knowledge at the theoretical level is essential.

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 which is fully acknowledged by all personnel of the institute who otherwise could not carry out this research. In fact, just to maintain the computational infrastructure, essential to carry out a high-quality and competitive research is not a simple task and without the support from the institution it would not have been possible. This is also thanks to the, often invisible, excellent technical staff that is responsible for keeping the whole computational framework adequately working. The research *memoir* that follows exemplifies the IQTCUB vitality, the considerable scientific production in research lines as different as drug design, heterogeneous catalysis, nanostructures, and atmospheric chemistry clearly demonstrates the growing impact of our research. The past year, 2014, also represents the starting of a new cycle since it constitutes the start of my second and last term as IQTCUB Director. In the years to come we hope that the IQTCUB project will continue deserving the support of our university and thus be able to further improve the scientific quality already recognized by external peer review evaluation in 2013 with the report available at the institute recently renewed web page.

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 76 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
Reigada Sanz	Ramón	Physical Chemistry

Other categories (Professors Associats)

Gómez Coca	Silvia	Inorganic Chemistry
Prats García	Hèctor	Physical 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

Juan de la Cierva contract

Jover Modrego	Jesús	Inorganic Chemistry

Beatriu de Pinós-Marie Curie

Cirera Fernández	Jordi	Inorganic Chemistry

Beatriu de Pinós

Albareda Piquer	Guillem	IQTCUB
Jornet Somoza	Joaquim	Physical Chemistry

Ramón y Cajal contract

Ribas Ariño	Jordi	Physical Chemistry
Viñes Solana	Francesc	Physical Chemistry

Other

Álvarez Falcón	Leny	Physical Chemistry
Chul Ko	Kyoung	Physical Chemistry
Kovács	Gábor	Physical Chemistry
Pastor del Campo	Isabel	Physical Chemistry

Ph D students

FPI (Associated with Ministerio Research Grants)

Aguilar Fargas	Javier	Physical Chemistry
Alcon Rovira	Isaac	Physical Chemistry
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
Vela Llausi	Sergi	Physical Chemistry
Vilà Casanova	Arnau	Physical Chemistry

FPU (Spanish Ministerio Program)

Capdevila Cortada	Marçal	Physical Chemistry
Kozlov	Sergey M.	Physical Chemistry
Mondelo Martell	Manel	Physical Chemistry
Rojas Cervellera	Victor	Organic Chemistry

UB own program

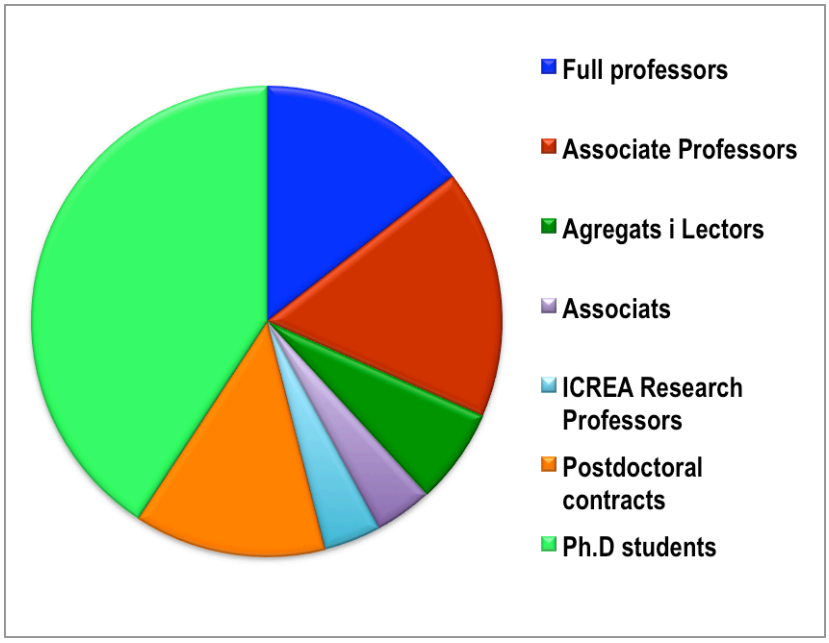
Fumanal Quintana	Maria	Physical Chemistry
Lamiel Garcia	J. Oriol	Physical Chemistry
Raich Armendáriz	Lluís	Organic Chemistry

FI (Catalan Government Program)

López Marne	Estefanía	Physical Chemistry

Other funding

Alonso Benito	Gerard	Physical Chemistry
Amoza Dávila	Martín	Inorganic Chemistry
Balcells Nadal	Cristina	Physical Chemistry
Blancafort Jorquera	Miquel	Physical Chemistry
Demiroglu	Ilker	Physical Chemistry
Figueroba Sánchez	Alberto	Physical Chemistry
Iglesias Fernández	Javier	Organic Chemistry
Martín Rodríguez	Alejandro	Inorganic Chemistry
Maxwell Villacorta	Lindley	Inorganic Chemistry
Morales Martínez	Roser	Inorganic Chemistry
Notario Estévez	Almudena	Physical Chemistry
Pueyo Bellafont	Noelia	Physical Chemistry
Reta Mañeru	Daniel	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, three 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*
Raul Porcel Martínez	*System Administrator*
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 other two machines of 9.000 KW.

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 360.000 €)

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

23 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)

5 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 30.000 €)

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

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

Processors..... 3230 CPUs

Memory.....21688 GB RAM

Calculation disk capacity ..... 174 TB

Data user disk capacity ..... 32 TB

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

2.100.000 €*

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

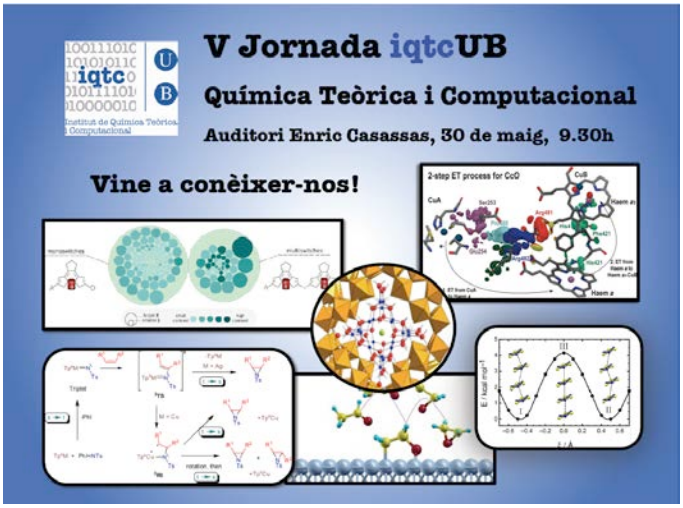
One of the clusters for intensive computation at IQTCUB

II. IQTCUB ACTIVITIES

II.1 GENERAL ACTIVITIES

Next, a description of activities and actions promoted by IQTCUB through 2014 is provided.

a. 5th IQTCUB workshop. This one-day workshop aimed at the dissemination of the research done at the IQTCUB took place on May 30th, 2014. The IQTCUB members and internationally acknowledged speakers present the most recent work. This year we highlight the participation of Prof. Denis Jacquemin from *Université de Nantes,* Prof. Feliu Maseras from *ICIQ*, Prof. Víctor Guallar from *BSC-IRB*, Dr. Xavier López from *Universitat Rovira i Virgili*, and Dr. Francesc Viñes and Dr. Sergi Vela from Universitat de Barcelona. The IQTCUB assigned a budget to cover the traveling expenses of Prof. Jacquemin as well as the catering service offered to all participants. Total cost: 1300 €



b. *Promotion and encouragement of research*. This year the IQTCUB has offered a total of three contracts (around 2000 € per contract) aimed to help students to initiate a scientific career. These contracts are addressed to students about to end the degree and aimed to cover a six month period to facilitate the student to pursue an official Master at UB as well as collaborating in some of the research projects of the IQTCUB groups. The contracts have been awarded to Mr. Alejandro Martín Rodríguez, Ms. Alba Nin Hill and Ms. Mireia Via Nadal. Total cost: 6140 €

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 2014 edition has been the fourth one and has been very successful with over 30 students requesting to participate. The course took place from June 25th to July 1st with an attendance of 27 students.

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, 2nd-8th with an attendance of 16 students.

IQTCUB has covered catering expenses for both courses on Computational Chemistry with a total cost of 670 €.

Picture corresponding to the "Introductory Course in Computational Chemistry" that took place in June 2014 at the Chemistry Faculty of the *Universitat de Barcelona*.

Picture corresponding to the "Advanced Course in Computational Chemistry" that took place in July 2014 at the Chemistry Faculty of the *Universitat de Barcelona*.

II.2 IQTCUB SEMINARS AND CONFERENCES

Thirteen seminars have been organized by IQTCUB during 2014.

1. **Prof. Roy Johnston** (University of Birmingham) UK

   Combining Theory and Experiment to Determine the Structures of Gas Phase Metal Clusters

   February 25th, 2014

2. **Dr. Marcos Fernández-García** (Consejo Superior de Investigaciones Científicas) Spain

   Multitechnique approach to Heterogeneous Catalysis: from preparation to reaction

   February 27th, 2014

3. **Dr. Joaquim Jornet-Somoza** (Université Montepellier) France

   The role of pyramidalisations, torsion and stretching in the V←N and R(3s)←N photodynamics of ethylene

   February 28th, 2014

4. **Prof. Jaakko Akola** (University of Tampere) Finnland

   Au nanoclusters as superatoms: DFT and MD simulations

   March 7th, 2014

5. **Dr. Martijn Zwijnenburg** (University College London) UK

   A Computational Perspective on the Photochemistry of Materials

   March 31st, 2014

6. **Prof. Juan E. Peralta** (Michigan University) USA

   Magnetic Exchange Couplings in Transition Metal Complexes from First-Principles Calculations

   June 2nd, 2014

7. **Federico Brivio** (University of Bath) United Kingdom

   DFT calculations for Perovskites Solar Cells

June 13th, 2014

8. **Dr. Nisanth N. Nair** (Indian Institute of Technology Kanpur) India

   QM/MM Modelling of Catalytic Reactions: Developments and Applications

   July 3rd, 2014

9. **Prof. Dr. Hans-Peter Steinrück** (Friedrich-Alexander University Erlangen-Nuremberg) Germany

   Surface Chemistry of Hydrocarbons - from Small Molecules to Graphene and Liquid Organic Hydrogen Carriers

   July 17th, 2014

10. **Prof. Carmen Domene** (Kings College London) UK

    Studies of ion conduction through cell membranes using free energy methods

    September 18th, 2014

11. **Dr. David Balcells** (University of Olso) Norway

    DFT Studies on the Dark Side of Catalysis: Active Species Generation and Catalyst Degradation

    December 3rd, 2014

12. **Dr. Jon M. Maxtain** (University of the Basque Country) Spain

    Novel Solid Phases by Self-Assembling of Nanoclusters

    December 12th, 2014

13. **Dr. Sergi Ruiz-Barragan** (Institute for Molecular Science) Japan

    Photophysics of fulvene under the non-resonant Stark effect. Shaping the conical intersection seam

    December 16th, 2014

II.3 IQTCUB INVITED RESEARCHERS

During 2014, a total of six researchers from all over the world have spent some time at the IQTCUB collaborating in different research projects.

1. **Miroslava Nedyalkova** (invited visitor)
   University of Sofia, Bulgaria
   February, 2014

2. **Ichraf Oueslati** (invited visitor)
   Université Pierre et Marie Curie, Paris, France
   March-July, 2014

3. **Alexander S Mikhailov** (invited visitor)
   Fritz Haber Institute, Germany
   June, 2014

4. **Laura Pitulice** (invited visitor)
   West University of Timisoara, Romania
   September, 2014

5. **Mikhail Polynski** (invited visitor)
   Institute of Organic Chemistry, Russian Academy of Sciences, Moscow, Russia
   September-October, 2014

6. **David Balcells** (invited visitor)
   University of Oslo, Finnland
   November-December, 2014

III. SCIENTIFIC ACTIVITY OF IQTCUB MEMBERS

III.1 HIGHLIGHTS FROM MOST RELEVANT RESULTS

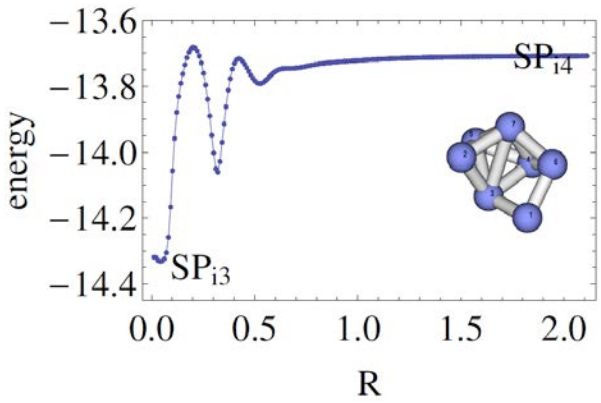
Here some of the most relevant results corresponding to every IQTCUB main research line are presented.

LINE 1. METHODS, ALGORITHMS AND COMPUTATIONAL TOOLS DEVELOPMENT

Locating saddle points of any index on potential energy surfaces by the generalized gentlest ascent dynamics

W. Quapp, J. M. Bofill

Theor. Chem. Acc., *133* (2014) 1510.



Energy profile over an index-4-GAD trajectory beginning at a LJ_7-SP of index 3, to a LJ_7-SP of index 4. R is an abstract 'reaction coordinate', the inlet is the shape of the SPi_4.

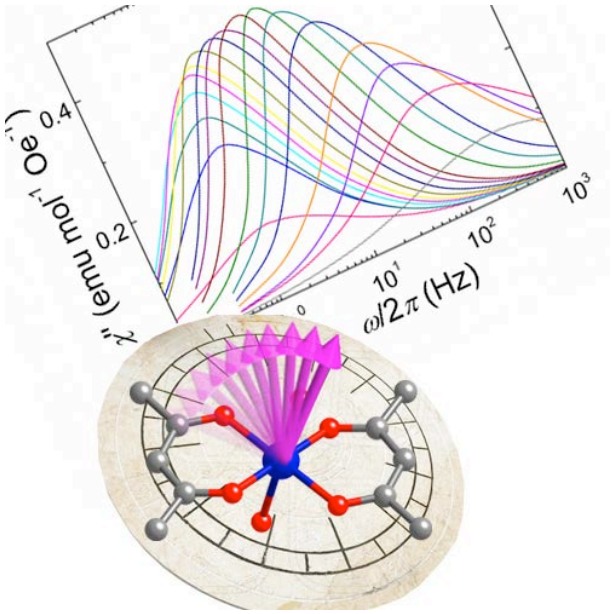
The system of ordinary differential equations for the method of the gentlest ascent dynamics (GAD) has been derived which was previously proposed [W. E and X. Zhou, Nonlinearity 24, 1831 (2011)]. For this purpose we use diverse projection operators to a given initial direction. Using simple examples we explain the two possibilities of a GAD curve: it can directly find the transition state by a gentlest ascent, or it can go the roundabout way over a turning point and then find the transition state going downhill along its ridge. An outlook to generalised formulas for higher order saddle-points is added.

LINE 2. COMPUTATIONAL MATERIALS SCIENCE

Origin of slow magnetic relaxation in Kramers ions with non-uniaxial anisotropy

S. Gómez-Coca, A. Urtizbarea, E. Cremades, P. J. Alonso, A. Camón, E. Ruiz, F. Luis

Nature Commun., *5* (2014) 4300.

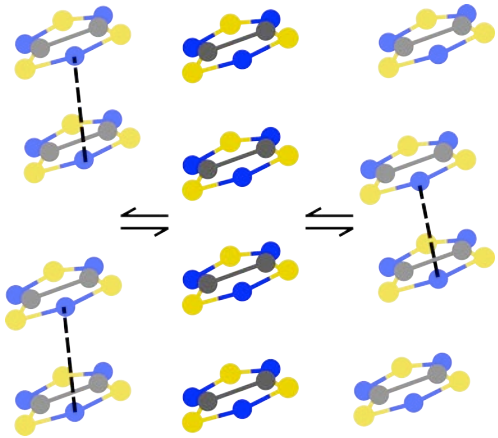


Quantitative first-principles calculations on the Kramers Co^{II} ion in the $[Co(acac)_2(H_2O)_2]$ complex show that the slow magnetic relaxation in this and similar systems is a general consequence of time-reversal symmetry that hinders direct spin-phonon processes. This conclusion applies regardless of the sign of the zero-field splitting parameters associated to the two forms of magnetic anisotropy, *easy axis* and *easy field* magnetization. The hyperfine interaction between electronic and nuclear spins opens paths for magnetic relaxation that would otherwise be forbidden by time reversal symmetry and uncovers a promising strategy for the design and achievement of atom-size magnetic memories.

The key role of vibrational entropy in the phase transitions of dithiazolyl-based bistable magnetic materials

S. Vela, F. Mota, M. Deumal, R. Suizu, Y. Shuku, A. Mizuno, K. Awaga, M. Shiga, J. J. Novoa, J. Ribas-Arino

Nature Commun., *5* (2014) 4411.



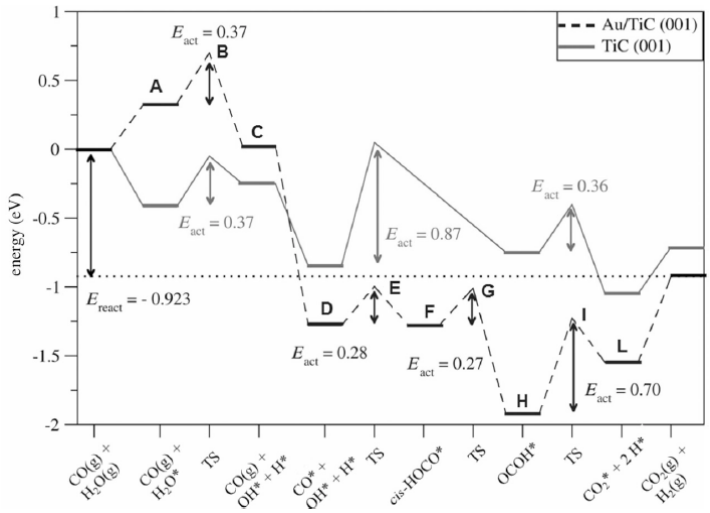
Pair-exchange dynamics in the TTTA material

The neutral radical 1,3,5-trithia-2,4,6-triazapentalenyl (TTTA) is a prototype of molecule-based bistable materials. TTTA crystals undergo a first-order phase transition between their low-temperature diamagnetic and high-temperature paramagnetic phases, with a large hysteresis loop that encompasses room temperature. Here, based on ab initio molecular dynamics simulations and new X-ray measurements, we uncover that the regular stacking motif of the high-temperature polymorph is the result of a fast intra-stack pair-exchange dynamics, whereby TTTA radicals continually exchange the adjacent TTTA neighbour (upper or lower) with which they form an eclipsed dimer. Such unique dynamics, observed in the paramagnetic phase within the whole hysteresis loop, is the origin of a significant vibrational entropic gain in the low-temperature to high-temperature transition and thereby it plays a key role in driving the phase transition. This finding provides a new key concept that needs to be explored for the rational design of novel molecule-based bistable magnetic materials.

Charge Polarization at a Au-TiC Interface and the Generation of Highly Active and Selective Catalysts for the Low-Temperature Water-Gas Shift Reaction

J.A. Rodriguez, P.J. Ramirez, G.G. Asara, F. Viñes, J. Evans, P. Liu, J.M. Ricart, F. Illas

Angew. Chem. Int. Ed., *53* (2014) 11270.



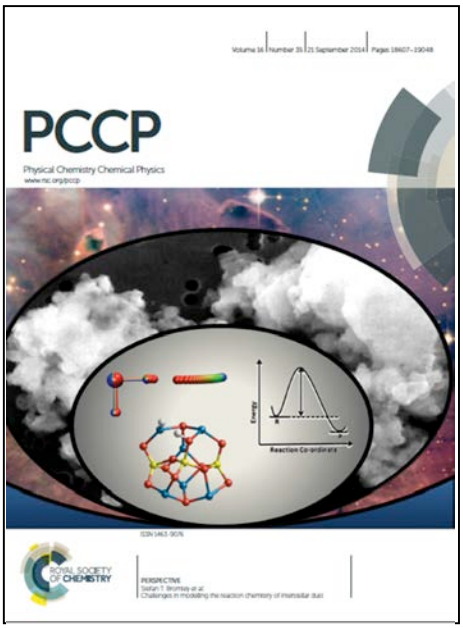
Energy derived from DFT calculations for the WGS reaction on clean TiC(001) and Au_4/TiC(001). TS = transition state.

Au atoms in contact with TiC(001) undergo a significant charge polarization. The strong metal–support interactions make Au/TiC(001) an excellent catalyst for the low-temperature water–gas shift (WGS), with turnover frequencies orders of magnitude larger than those observed for conventional metal/oxide catalysts such as Cu/ZnO. DFT calculations indicate that the WGS reaction follows an associative mechanism with HOCO as a key intermediate, showing how the synergy of Au/TiC(001) and the charge polarization is at the hearth of the different catalytic activity of Au/TiC(001) compared to TiC(001).

Challenges in modelling the reaction chemistry of interstellar dust

S. T. Bromley, T. P. M. Goumans, E. Herbst, A. P. Jones and B. Slater

Phys. Chem. Chem. Phys. (Perspective), *74* (2014) 58.

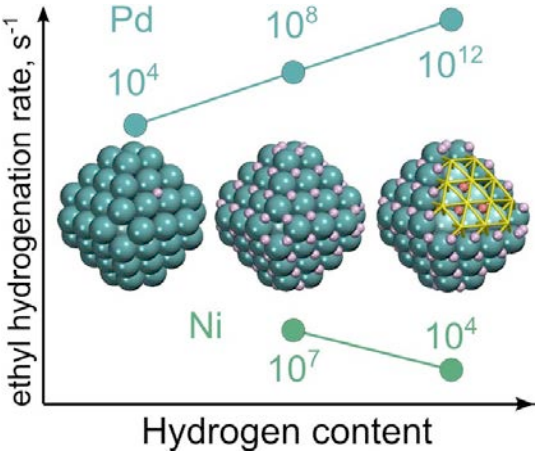


The challenges in modelling the reaction chemistry of interstellar dust are concisely reviewed.

How absorbed hydrogen affects catalytic activity of transition metals

H.A. Aleksandrov, S.M. Kozlov, S. Schauermann, G.N. Vayssilov, K.M. Neyman

Angew. Chem. Int. Ed., 53 (2014) 13371.

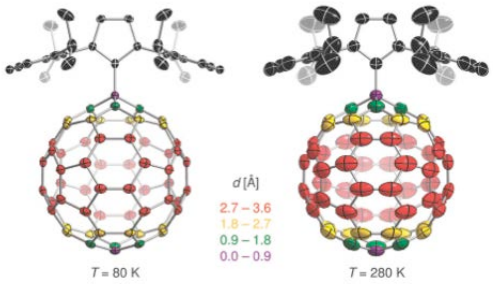


Understanding hydrogenation on transition metals: Subsurface hydrogen, H_{sub}, is shown to significantly influence the stability and the reactivity of the adsorbed hydrogen on transition metals in two different ways. Very surprisingly, density functional calculations on a representative reaction, ethyl hydrogenation, show that it is accelerated on Pd and Pt, but slowed down on Ni and Rh in the presence of H_{sub}.

A Fullerene-Carbene Adduct as a Crystalline Molecular Rotor: Remarkable Behavior of a Spherically-Shaped Rotator

E. Lorbach, E. Maverick, A. Carreras, P. Alemany, G. Wu, M.A. Garcia-Garibay, G.C. Bazan

Phys. Chem. Chem. Phys., *16* (2014) 12980.



Thermal displacement ellipsoids at 80 and 280 K indicate the presence of a rapid rotation of the C_{60} fragment around the C-C bond joining it to the carbene at high temperature. The color code indicates the distance of the atoms on the fullerene to the rotation axis.

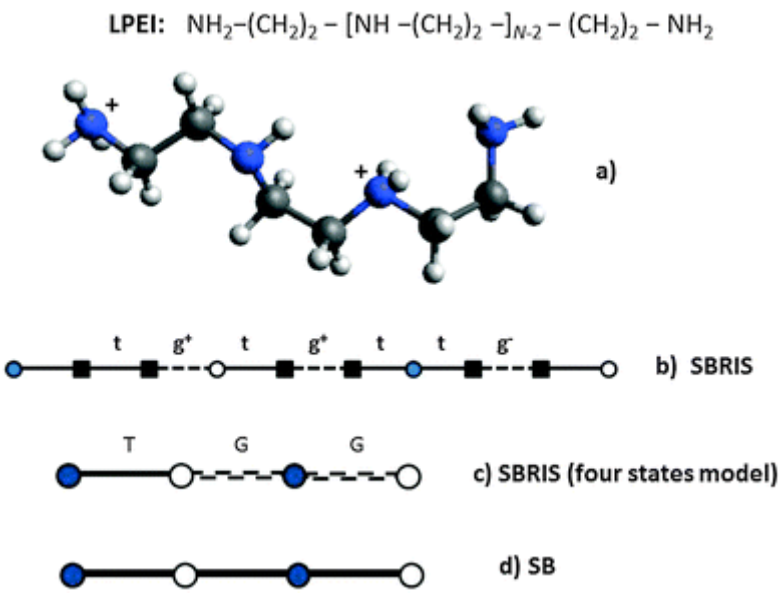
A new fullerene structure was recently obtained from the reaction of a N-heterocyclic carbene and C_{60}. The molecular features of the zwitterionic adduct can be described as a molecular rotor with the fullerene cage acting as the rotator that spins about one distinct axis given by its C–C single bond linkage with the imidazolium heterocycle stator. Variable temperature single-crystal x-ray diffraction experiments (80 K < T < 480 K) carried out to investigate the rotational dynamics of the fullerene group revealed atomic displacement parameters consistent with fast rotation of the highly symmetric fullerene in the solid state, whereas the imidazolium unit remains in a fixed position and therefore represents the stator. DFT and semiempirical calculations were applied to get insight into the profile of the rotational potential of the fullerene unit, particularly considering interactions with the neighboring molecules in the crystal lattice. The results indicate that the crystal environment leads to the presence of one lowest energy minimum that is connected to seven others that are slightly higher in energy through rotational barriers of approximately 1.5–2.5 kcal mol^{-1}.

LINE 3. COMPUTATIONAL BIOCHEMISTRY AND *SOFT MATTER*

Coupling of conformational and ionizatin equilibria in linear poly(ethylenimine): a study based on site binding/rotational isomeric state (SBRIS) model

J.L. Garcés, S. Madurga, M. Borkovec

Phys. Chem. Chem. Phys., *16* (2014) 4626.



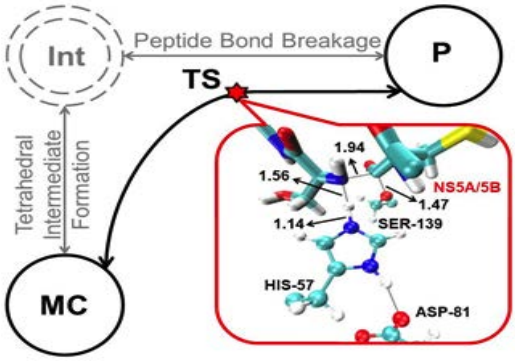
Possible ionization and the conformational state of a linear polyethyleneimine (LPEI) oligomer with four amine groups. The conformation and charge distribution of the polyelectrolyte is treated at different levels.

The conformational and ionization properties of linear polyethylenimine are studied by combining the site binding model (SB) with the rotational isomeric state (RIS) model, developed by Flory to calculate the conformational properties of neutral linear molecules. The resulting approach (the SBRIS model) is used to rationalise the experimental polyethylenimine titration curves. By fitting the experimental macroconstants, conformational and binding parameters are obtained. The obtained values are consistent with previous binding and structural information. In order to account for excluded volume and long-range electrostatic interactions, Monte Carlo simulations are performed. The results indicate that at high ionic strengths, long-range interactions have a very limited impact on the titration curves. However, for long chains, they have a significant influence on the radius of gyration.

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 really exist?

J. A. Martínez-González, M. González, L. Masgrau, R. Martínez

ACS Catal. in press (dx.doi.org/10.1021/cs5011162).



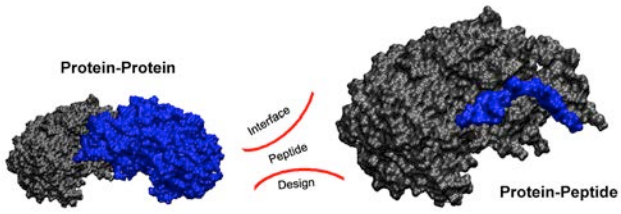
Concerted acylation mechanism found for the reaction of the NS3/NS4A serine protease and the NS5A/5B substrate, compared with the generally proposed two-step mechanism. A molecular representation of the transition state characterized is also shown.

The SCC-DFTB/MM and EA-VTST/MT theoretical methods were used to analyze the mechanism and calculate the rate constant of the NS3/NS4A protease + NS5A/5B acylation reaction, which is very important in the vital cycle of the hepatitis C virus. A concerted reaction mechanism with a single transition state (TS) has been determined, in contrast with the proposed general two-steps serine protease acylation mechanism. This is related to the fact that the enzyme is particularly efficient for NS5A/5B. The acylation TS found here can be a good initial structure in the search of NS3/NS4A inhibitors based on TS analogs. Moreover, the calculated and experimental phenomenological free energy barriers only differ by 2.3 kcal mol^{-1} (although this leads to a significant discrepancy between calculated and experimental rate constants), and the rest of calculated kinetic parameters (kinetic isotopic effect (H/D), tunneling, and recrossing) agree with the expected behaviour for the studied reaction.

Design of an interface peptide as new inhibitor of humanglucose-6-phosphate dehydrogenase

C. Obiol-Pardo, G. Alcarraz-Vizánb, S. Díaz-Moralli, M. Cascante, J. Rubio-Martinez

Journal of Molecular Graphics and Modelling, *49* (2014) 110



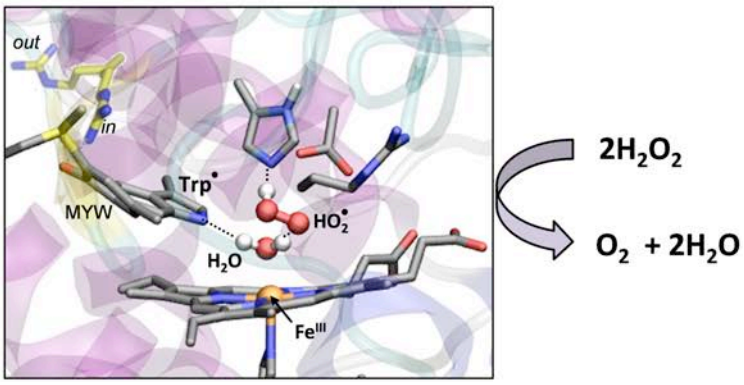
Design of interface peptides

Glucose-6-phosphate dehydrogenase (G6PDH) is an essential enzyme involved in the first reaction of the oxidative branch of the pentose phosphate pathway (PPP). Recently, G6PDH was suggested as a novel target protein for cancer therapy as one of the final products of the PPP, ribose-5-phosphate, is necessary for nucleic acid synthesis and tumor progression. After analyzing the protein–protein interface of the crystal structure of human G6PDH by means of molecular dynamics simulations, we designed six interface peptides based on the natural sequence of the protein. The three most promising peptides, as predicted by binding free energy calculations, were synthesized and one of them was confirmed as a novel inhibitor of human G6PDH in experimental assays. Together, the active peptide found and its suggested binding mode proposes a new strategy for inhibiting this enzyme and should aid the further design of novel, potent and non-peptidic G6PDH inhibitors.

An ionizable triptophane residue imparts catalase activity to a peroxidase core

P. C. Loewen, X. Carpena, P. Vidossich, I. Fita, C. Rovira

J. Am. Chem. Soc., *136* (2014) 7249. JACS Spotlight.



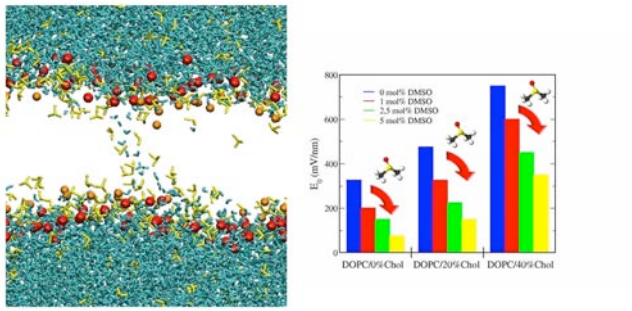
Enzyme intermediate determined by quantum mechanics/molecular mechanics (QM/MM) simulations.

When it comes to enzymes and hydrogen peroxide (H_2O_2), there are catalases and peroxidases. The former degrade hydrogen peroxide; the latter use it to oxidize other molecules. The heme-containing catalase-peroxidases (KatGs) perform both activities, but as the enzymes' active sites tend to resemble peroxidases (which have poor catalase activity), it has never been clear how they work. KatGs have a unique methionine-tryptophan-tyrosine (MWY) "covalent adduct" near the heme ring, as well as a critical arginine residue that alternates between "in" and "out" orientations. Using QM/MM calculations and x-ray crystallography, we demonstrate that the adduct tryptophan loses a proton during the catalytic cycle. We also propose an eight-step mechanism in which the MWY complex and mobile arginine act as an "electronic switch" that drives conversion of hydrogen peroxide to water and oxygen.

Effects of Dimethyl Sulfoxide on Lipid Membrane Electroporation

M.L. Fernández, R. Reigada

J. Phys. Chem. B, *118* (2014) 9306.



DMSO (yellow) facilitates the formation of electropores in the membrane and the passage of water molecules (cyan). This effects causes a reduction of the minimum electroporation field

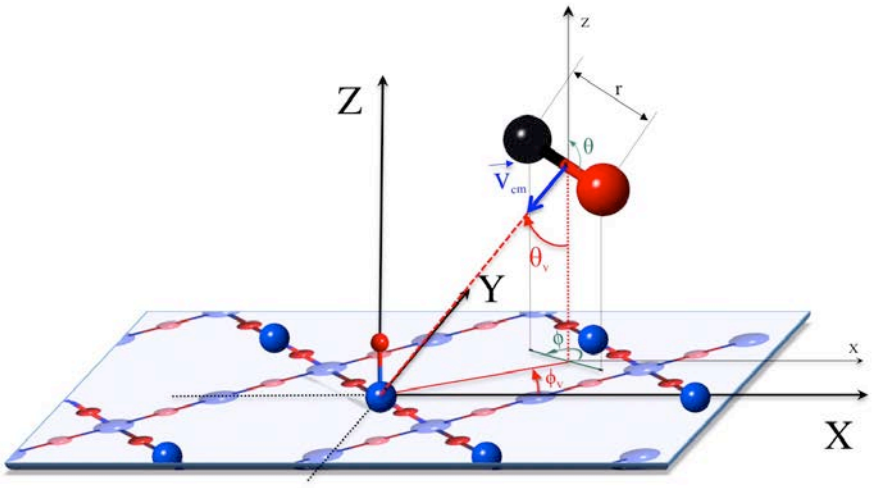
Pores can be generated in lipid membranes by the application of an external electric field or by the addition of particular chemicals such as dimethyl sulfoxide (DMSO). Molecular dynamics (MD) has been shown to be a useful tool for unveiling many aspects of pore formation in lipid membranes in both situations. By means of MD simulations, we have addressed the formation of electropores in cholesterol-containing lipid bilayers under the influence of DMSO. We show how a combination of physical and chemical mechanisms leads to more favorable conditions for generating membrane pores and, in particular, how the addition of DMSO to the medium significantly reduces the minimum electric field required to electroporate a lipid membrane. The strong alteration of membrane transversal properties and the energetic stabilization of the hydrophobic pore stage by DMSO provide the physicochemical mechanisms that explain this effect.

LINE 4. REACTIVITY AND REACTIONS DYNAMICS

ReaxFF molecular dynamics simulations of CO collisions on an O-preadsorbed silica surface

P. Gamallo, H.Prats, R.Sayós

J. Mol. Model. *20* (2014) 2160.



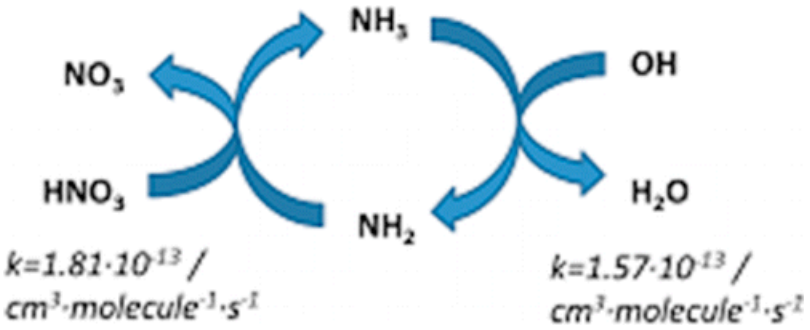
CO molecule interacting with an O-preadsorbed β-cristobalite (001) surface

A quasiclassical trajectory dynamics study was performed for carbon monoxide collisions over an oxygen preadsorbed β-cristobalite (001) surface. A reactive molecular force field (ReaxFF) was used to model the potential energy surface. The collisions were performed fixing several initial conditions: CO rovibrational states (v = 0-5 and j = 0, 20, 35), collision energies ($0.05 \leq E_{col} \leq 2.5$ eV), incident angles (θ_v = 0°, 45°) and surface temperatures (T_{surf} = 300 K, 900 K). The principal elementary processes were the molecular reflection and the non-dissociative molecular adsorption. CO_2 molecules were also formed in minor extension via an Eley-Rideal reaction although some of them were finally retained on the surface. The scattered CO molecules tend to be translationally colder and internally hotter (rotationally and vibrationally) than the initial ones. The present study supports that CO + O_{ad} reaction should be less important than O + O_{ad} reaction over silica for similar initial conditions of reactants, in agreement with experimental data.

Unexpected Reactivity of Amidogen Radical in the Gas Phase Degradation of Nitric Acid

J.M. Anglada, S. Olivella, A. Solé

J. Am. Chem. Soc., *136* (2014) 6834.



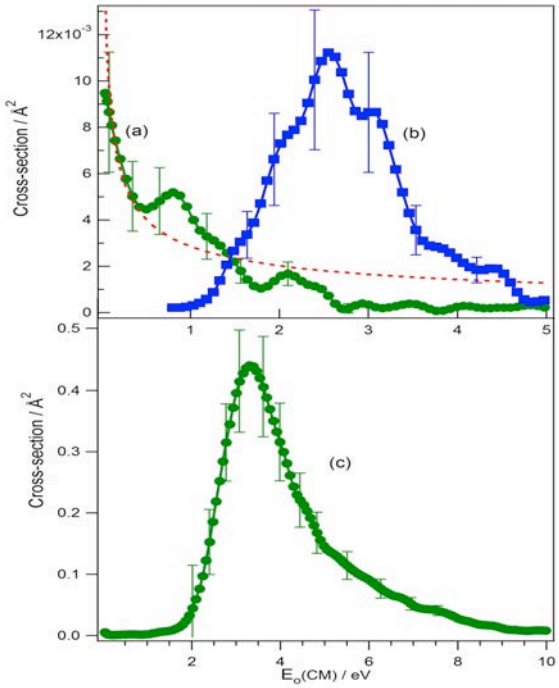
Catalytic cycle involving the oxidation of NH_3 by OH radical and the reaction between amidogen radical and nitric acid

The gas phase reaction between nitric acid and amidogen radical has been investigated employing high level quantum-mechanical electronic structure methods and variational transition state theory kinetic calculations. Our results show that the reaction proceeds through a *proton coupled electron transfer* mechanism with a rate constant of 1.81×10^{-13} $cm^3 \cdot molecule^{-1} \cdot s^{-1}$ at 298 K. This value is similar to the rate constants for the reactions of hydroxyl radical with either ammonia or nitric acid. An analysis of these data in the context of the chemistry of the atmosphere suggests that the amidogen radical, formed in the oxidation of ammonia by hydroxyl radical, reacts with nitric acid regenerating ammonia. On the basis of these findings, we propose a potential new catalytic-like cycle which couples the oxidation of ammonia by hydroxyl radical and the reaction of nitric acid with amidogen radical in the Earth's atmosphere.

Experimental guided ion beam and *ab initio* studies of the reactive processes in gas phase *i*-C_3H_7Br and *i*-C_3H_7OH collisions with potassium ions

E. López, J.M. Lucas, J. de Andrés, M. Albertí, J.M. Bofill, D. Bassi and A. Aguilar.

J. Chem. Phys., *141* (2014) 164310.



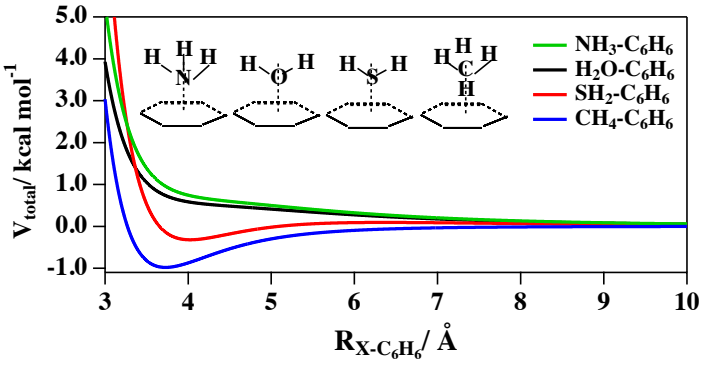
Cross-section CM energy dependences in K^+ + *i*-C_3H_7Br collisions for: (a) [K-*i*-$C_3H_7Br]^+$ adduct formation (●); (b) dehydrohalogenation reaction (■); (c) adduct decomposition reaction. Discontinuous line: LGS model (energies are given in the CM frame)

Collisions between K^+ and *i*-C_3H_7Br and *i*-C_3H_7OH molecules, all in their electronic ground state, have been studied in our laboratory in the 0.10-10.00 eV center of mass (CM) collision energy range, using the radiofrequency-guided ion beam (RF-GIB) technique. In K^+ + *i*-C_3H_7Br collisions $KHBr^+$ formation is observed and quantified, while the analogous KH_2O^+ formation by *i*-C_3H_7OH dehydration was hardly detected. Moreover, formation of the [K–*i*-$C_3H_7Br]^+$ and [K–*i*-$C_3H_7OH]^+$ adducts and their decomposition leading to $C_3H_7^+$ and KBr or KOH, respectively, have been observed. Absolute reaction cross-sections are measured as a function of the CM energy and the thermal rate constant at 303 K has been calculated for $KHBr^+$ formation. *Ab initio* structure calculations at the MP2 level gave information about the relevant features of the potential energy surfaces where reactions take place adiabatically for both systems and allowed a qualitative interpretation of the experimental data to be proposed.

Benzene-Hydrogen Bond (C_6H_6-HX) Interactions: The Influence of the X Nature on their Strength and Anisotropy

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

J. Phys. Chem. A, *118* (2014) 1651



H_2O-C_6H_6, SH_2-C_6H_6, NH_3-C_6H_6, and CH_4-C_6H_6
intermolecular interaction potentials for the represented molecular approaches

The intermolecular potential energy of the C_6H_6-SH_2 and C_6H_6−NH_3 dimers is formulated as combination of electrostatic and nonelectrostatic contributions. The relevant parameters, derived from molecular polarizability components, allow describing in a consistent way both size repulsion and dispersion attraction forces. The features of the most stable configurations predicted by the potential model have been compared with available ab initio and experimental data. Moreover, the strength of the C_6H_6−HX interaction has been analyzed by comparing the obtained results with the corresponding ones for the C_6H_6−H_2O and the C_6H_6−CH_4 systems, investigated previously with the same methodology. Information on the relative orientation of the partners, arising from the anisotropy of the intermolecular interaction, evaluated at different intermolecular distances, has been also obtained. Such information is crucial to evaluate sterodynamics effects in bimolecular collisions.

III.2 PUBLICATION LIST

ARTICLES

1. *Optical control of enzyme enantioselectivity in solid phase.*
A. Bautista-Barrufet, F. López-Gallego, V. Rojas-Cervellera, C. Rovira, M. A. Pericàs, J. M. Guisán, P. Gorostiza.
ACS Catal. *4* (2014), 1004.

2. *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 really exist?.*
J. A. Martínez-González, M. González, L. Masgrau, R. Martínez
ACS Catal. in press (dx.doi.org/10.1021/cs5011162).

3. *Hydrogen/Deuterium Exchange-Protected Oligomers Populated during A² Fibril Formation Correlate with Neuronal Cell Death*.
B. Serra-Vidal, L. Pujadas, D. Rossi, D. Soriano, S. Madurga, N. Carulla
ACS Chemical Biology *9* (2014), 2678.

4. *Combined inhibitor free-energy landscape and structural analysis reports on the mannosidase conformational coordinate.*
R. J. Williams, J. Iglesias-Fernández, J. Stepper, A. Jackson, A. J. Thompson, E. C. Lowe, J. M. White, H. J. Gilbert, C. Rovira, G. J. Davies, S. J. Williams.
Angew. Chem. Int. Ed. *53* (2014), 1087.

5. *Fluorocarbons modulate the coordination sphere of f-element complexes.*
S. Álvarez, B. Menjón
Angew. Chem. Int. Ed. *53* (2014), 2810.

6. *Combined structural snapshots and metadynamics reveal a substrate-guided front-face reaction for polypeptide GalNAc-transferase T2.*
E. Lira-Navarrete, J. Iglesias-Fernández, W. F. Zandberg, I. Compañón, Y. Kong, F. Corzana, B. M. Pinto, H. Clausen, J. M. Peregrina, D. Vocadlo, C. Rovira, R. Hurtado-Guerrero
Angew. Chem. Int. Ed. *53* (2014), 8206.

7. *Maximum Noble-Metal Efficiency in Catalytic Materials: Atomically Dispersed Surface Platinum.*
A. Bruix, Y. Lykhach, I. Matolínová, A. Neitzel, T. Skála, N. Tsud, M. Vorokhta, V. Stetsovych, K. Ševčíková, J. Mysliveček, R. Fiala, M. Václavů, K.C. Prince, S. Bruyère, V. Potin, F. Illas, V. Matolín, J. Libuda, K.M. Neyman
Angew. Chem. Int. Ed. *53* (2014), 10525.

8. *Charge Polarization at a Au-TiC Interface and the Generation of Highly Active and Selective Catalysts for the Low-Temperature Water-Gas Shift Reaction.*
J.A. Rodriguez, P.J. Ramirez, G.G. Asara, F. Viñes, J. Evans, P. Liu, J.M. Ricart, F. Illas
Angew. Chem. Int. Ed. *53* (2014), 11270.

9. *How absorbed hydrogen affects catalytic activity of transition metals.*
H.A. Aleksandrov, S.M. Kozlov, S. Schauermann, G.N. Vayssilov, K.M. Neyman
Angew. Chem. Int. Ed. *53* (2014), 13371.

10. *Dust in brown dwarfs and extra-solar planets. IV. Assessing TiO_2 and SiO nucleation for cloud formation modelling.*
G. Lee, C. Helling, H. Giles, S. T. Bromley
Astronomy and Astrophysics, Accepted, in press.

11. *Electroporation of heterogeneous lipid membranes.*
R. Reigada
Biochim. et Biophys. Acta *1838* (2014), 814.

12. *Effect of crowding by Dextrans in enzymatic reactions.*
I. Pastor, C. Balcells, L. Pitulice, E. Vilaseca, S. Madurga, A. Isvoran, M. Cascante, F. Mas
Biophys. Chem. *185* (2014), 8.

13. *Atomic Level Rendering of DNA-Drug Encounter*.
M. F. Lucas, I. Cabeza de Vaca, R. Takahashi, J. Rubio-Martinez, V. Guallar
Biophys. J.*105* (2014), 421.

14. *Identifying atomic sites in N-doped pristine and defective graphene from ab initio core level binding energies.*
N.P. Bellafont, D.R. Mañeru, F. Illas
Carbon *76* (2014), 155.

15. *On the importance of thermal effects and crystalline disorder in the magnetism of benzotriazinyl-derived organic radicals.*
M. Fumanal, S. Vela, J. Ribas-Arino, J.J. Novoa
Chem. Asian. J. *9* (2014), 3612.

16. *Enantioselective preparation of δ-valerolactones using horse liver alcohol dehydrogenase.*
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Phys. Chem. Chem. Phys. *16* (2014) 4626.

112. *Hydrogen storage on metal oxide model clusters using density-functional methods and reliable van der Waals corrections.*
J. Gebhardt, F. Viñes, P. Bleiziffer, W. Hieringer, A. Görling.
Phys. Chem. Chem. Phys. *16* (2014), 5382.

113. *Understanding the effect of vibrational excitation in reaction Dynamics: Ne + H_2^+ (v=0-17, j=1) → NeH^+ + H, Ne + H^+ + H proton transfer and dissociation cross sections.*
P. Gamallo, R. Martínez, José D. Sierra, M. González.
Phys. Chem .Chem. Phys. *16* (2014), 6641.

114. *O vacancies on steps on CeO_2(111) surface.*
S.M. Kozlov, K.M. Neyman
Phys. Chem. Chem. Phys. *16* (2014), 7823.

115. *A study on adatom transport through (√3×√3)-R30 degrees-CH_3S self-assembled monolayers on Au(111) using first principles calculations.*
D. Paulius, D. Torres, F. Illas, W.E. Archibald
Phys. Chem. Chem. Phys. *16* (2014), 10850.

116. *A Fullerene-Carbene Adduct as a Crystalline Molecular Rotor: Remarkable Behavior of a Spherically-Shaped Rotator*
A. Lorbach, E. Maverick, A. Carreras, P. Alemany, G. Wu, M.A. Garcia-Garibay, G.C. Bazan
Phys. Chem. Chem. Phys. *16* (2014), 12980.

117. *The bending machine: CO_2 activation and hydrogenation on δ-MoC(001) and β-Mo_2C(001) surfaces.*
S. Posada-Pérez, F. Viñes, P.J. Ramirez, A.B. Vidal, J.A. Rodriguez, F. Illas
Phys. Chem. Chem. Phys. *16* (2014), 14912.

118. *Atmospheric formation of the NO3 radical from gas-phase reaction of HNO3 acid with the NH2 radical: proton-coupled electron-transfer versus hydrogen atom transfer mechanisms.*
J.M. Anglada, S. Olivella, A. Solé
Phys. Chem. Chem. Phys. *16* (2014) 19437.

119. *Line defects and induced doping effects in graphene, hexagonal boron nitride and hybrid BNC.*
N. Ansari, F. Nazari, F. Illas
Phys. Chem. Chem. Phys. *16* (2014), 21473.

120. *Potential energy surfaces and quasiclassical trajectory study of the O + H_2^+ → OH^+ + H, OH + H^+ proton and hydrogen atom transfer reactions and isotopic variants (D_2^+, HD^+).*
M. Paniagua, R. Martínez, P. Gamallo, M. González
Phys. Chem. Chem. Phys. *16* (2014), 23594.

121. *DFT studies of oxygen dissociation on the 116-atom platinum truncated octahedron particle.*
P.C. Jennings, H.A. Aleksandrov, K.M. Neyman, R.L. Johnston
Phys. Chem. Chem. Phys. *16* (2014), 26539.

122. *Insights into the crystal-packing effects on the spin crossover of $[Fe^{II}(1\text{-bpp})]^{2+}$-based materials.*
S. Vela, J.J. Novoa, J. Ribas-Arino
Phys. Chem. Chem. Phys. *16* (2014), 27012.

123. *Trends in the adsorption and reactivity of hydrogen on magnesium silicate nanoclusters.*
I. Oueslati, B. Kerkenia and S. T. Bromley
Phys. Chem. Chem. Phys. Accepted, in press.

124. *Electronic structure and anion ordering in $(TMTSF)_2ClO_4$ and $(TMTSF)_2NO_3$: a first principles study*
P. Alemany, J.P. Pouget, E. Canadell
Phys. Rev. B *89* (2014), 155124.

125. *Charge density wave – metal coexistence in the quasi-one dimensional organic conductor $TTF[Ni(dmit)_2]_2$.*
W. Kaddour, H. Raffy, M. Monteverde, P. Auban-Senzier, J.-P. Pouget, C.R. Pasquier, P. Alemany, E. Canadell, L. Valade
Phys. Rev. B *89* (2014), 205132.

126. *Correlated Electron-Nuclear Dynamics with Conditional Wave Functions.*
G. Albareda, H. Appel, I. Franco, A. Abedi, Á. Rubio.
Phys. Rev. Lett. *113* (2014), 083003.

127. *A molecular dynamics simulation of hydrogen atoms collisions on an H-preadsorbed silica surface.*
M. Rutigliano, P. Gamallo, R.Sayós, S. Orlandini, M. Cacciatore
Plasma Sources Science and Technology *23* (2014), 045016.

128. *The effect of tensile stress on the conformational free energy landscape of disulfide bonds*.
P. Anjukandi, P. Dopieralski, J. Ribas-Arino, D. Marx
PLOS One *9* (2014), e108812.

129. *Theoretical approach to the structure, energy and electronic spectroscopy of O@(^{4}He)$_N$ doped nanodroplets.*
A. Vilà, M. González, R. Mayol, M. Paniagua.
RSC Adv. *4* (2014), 44972.

130. *Multi-scale theoretical investigation of molecular hydrogen adsorption over graphene:coronene as a case.*
M.B. Yeamin, N. Faginas-Lago, M. Albertí, I.G. Cuesta, J. Sánchez-Marín, A. Sánchez
RSC Advances *4* (2014), 54447.

131. *A DF-vdW study of the CH_4 adsorption on different Ni surfaces.*
S. González, F. Viñes, J.F. Garcia, Y. Erazo, F. Illas
Surf. Sci. *625* (2014), 64.

132. *Theoretical and computational investigation of meta-phenylene as ferromagnetic coupler in nitronyl nitroxide diradicals.*
A.K. Pal, D. Reta-Mañeru, I.A. Latif, I.D.R. Moreira, F. Illas, S.N. Datta
Theor. Chem. Acc. *133* (2014), 1472.

133. *Locating Saddle Points of any Index on Potential Energy Surfaces by the Generalized Gentlest Ascent Dynamics.*
W. Quapp, J. M. Bofill
Theor. Chem. Acc. *133* (2014), 1510.

134. *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., (2014) Accepted, in press.

BOOK CHAPTERS AND PROCEEDINGS

1. *Theoretical and Computational Aspects of Magnetic Organic Molecules.*
S.N. Datta, C.O. Trindle, F. Illas
Theoretical and Computational Aspects of Magnetic Organic Molecules (2014) (Imperial College Press, World Scientific Publishing, Londres)

2. *Chemical bonding in solids.*
P. Alemany, E. Canadell
The Nature of the Chemical Bond Revisited, G. Frenkin, S. Shaik, Eds. (2014) 445 (Wiley-VCH, Weinheim)

3. *Car-Parrinello simulations of chemical reactions in proteins.*
C. Rovira
Protein Modelling (2014) 51 (Springer, Switzerland)

III.3 OTHER ACTIVITIES

DOCTORALS THESES 2014

1. *Computational modeling of heterogeneous catalysts based on platinum and cerium oxide*
   Albert Bruix Fusté
   Facultat de Química, Universitat de Barcelona
   February 2014

2. *Effect Dimensionality and Polymorphism on the properties of ZnO*
   Ilker Demiroglu
   Facultat de Química, Universitat de Barcelona
   February 2014

3. *Estudi experimental i teòric de la dinàmica de les reaccions ió-molècula*
   Javier Aguilar Fargas
   Facultat de Química, Universitat de Barcelona
   March 2014

4. *Long, multicenter bonding present in radical···radical interactions: a computational study*
   Marçal Capdevila Cortada
   Facultat de Química, Universitat de Barcelona
   July 2014

5. *Elucidating catalytic mechanisms in carbohydrate-active enzymes by means of ab initio molecular dynamics simulations*
   Javier Iglesias Fernández
   Facultat de Química, Universitat de Barcelona
   September 2014

6. *Computational modeling of molecular magnetic materials*
   Sergi Vela Llausí
   Facultat de Química, Universitat de Barcelona
   September 2014

THESES PRESENTED AT OTHER UNIVERSITIES AND COSUPERVISED BY MEMBERS OF IQTCUB

7. *Computational study of nanoparticles: the effect of metal ions, sovent and citric acid*
   Miroslava Nedyalkova
   Faculty of Chemistry and Pharmacy, University of Sofia
   March 2014

8. *Spin Crossover Mechanisms unraveled by Theory. Towards the design of new materials*
Andrii Rudavskyi
Facultat de Química, University of Groningen
September 2014

9. *Transition metal carbides as active phase and as support in catalysis: Insights from first principles theoretical modelling*
Gian Giacomo Asara
Facultat de Química, Universitat Rovira i Virgili
October 2014

MASTERS THESES 2014

1. *Enzyme Size as a Modulator of Macromolecular Crowding in Enzyme Kinetics: A Comparative Study*
Cristina Balcells Nadal
Facultat de Química, Universitat de Barcelona
July 2014

SCIENTIFIC CONFERENCES AND MEETINGS 2014

VIII Encuentro Franco-Español de Química y Física del Estado Sólido
Castellón, (Spain)

Cartography of the Van der Waals Territory
S. Álvarez

Special invited lecture at the *Dr. Barbara Mez-Starck Prizes for the Best Master Graduates* ceremony
Universität Ulm, Ulm (Germany)

Pseudosymmetry, nested symmetries and latent symmetry in the molecular world
S. Álvarez

Escuela de Verano sobre Historia de la Química
Universidad de La Rioja, Logroño (Spain)

La identidad y los atributos del átomo, antes y después de Bohr
S. Álvarez

16ª Reunión Bienal del Grupo Especializado de Química Inorgánica - QIES2014
Almería (Spain)

Imanes unimoleculares con anisotropía de tipo plano fácil
E. Ruiz

10th Congress of the World Association of Theoretical and Computational Chemists - WATOC 2014
Santiago de Chile (Chile)

Mononuclear easy-plane Single Molecule Magnets: A theoretical study
E. Ruiz, S. Gómez-Coca, E. Cremades

7th European School on Molecular Nanoscience - ESMolNa
Gandía (Spain)

Switching magnetoresistance in a Single-Molecule device at room temperature
E. Ruiz

Challenges in Inorganic and Materials Chemistry - ISACS13
Chartered Accountants House, Dublin (Ireland)

Copper-catalyzed trifluoromethylation of aryl iodides with CF_3SiEt_3: Computational insights
J. Jover

Understanding single-molecule magnets behaviour of mononuclear first-row transition metal complexes
S. Gómez Coca

XXXII Reunión del Grupo Especializado de Química Organometálica - GEQO XXXII
Universitat Rovira i Virgili, Tarragona (Spain)

Copper-catalyzed trifluoromethylation of aryl iodides with CF_3SiEt_3: Computational insights
J. Jover

The 2nd International Symposium for Young Chemists on Stimuli-Responsive Chemical Species for the Creation of Functional Molecules
Osaka University, Osaka (Japan)

The key role of second order phase transitions in dithiazolyl-based switchable magnetic materials
J. Ribas

AIAA Science and Technology Forum and Exposition 2014: 52nd Aerospace Sciences Meeting
National Harbor, Maryland (USA)

Phys4EntryDB: a database for state-to-state kinetics of planetary atmospheres
A. Laricchiuta, I. Armenise, M. Cacciatore, R. Celiberto, F. Esposito, P. Gamallo, A. Laganà, V. Laporta, A. Lombardi, S. Orlandini, F. Pirani, M. Rutigliano, R.Sayós, J.Tennyson, M. Capitelli

9th Congress on Electronic Structure: Principles and Applications. ESPA2014
Badajoz (Spain)

Kinetic Monte Carlo simulation of water-gas shift reaction on Cu(111)
H. Prats, L. Álvarez, F. Illas, R. Sayós

Spin Crossover in Fe(II) Materials
C. Sousa

Triplet-Singlet Gap Engineering in High Spin Ground State Alternant Hydrocarbon Diradicals
D. Reta-Mañeru, I.d.P.R. Moreira, F. Illas

The chemistry of the Titan's atmosphere
E. López, D. Ascenzi, J.M. Bofill and A. Aguilar

International Symposium Frontiers in surface and materials science: Theory and Practice
Universitat de Barcelona (Spain)

Organizing Committee
F. Viñes
C. Sousa
K.M. Neyman

Kinetic Monte Carlo study of water-gas shift reaction on copper (111) surface
H. Prats, L. Álvarez, F. Illas, R. Sayós

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

Absorption Spectrum of $[Fe(bpy)_3]^{2+}$: Beyond the Static Approach
A. Domingo, C. Sousa, C. de Graaf

5th international meeting on Atomic and Molecular Physics and Chemistry (IMAMPC 2014)
Salamanca (Spain)

Quantum dynamic effects of $O + H_2^+ \rightarrow OH^+ + H$, $OH + H^+$. Influence of nonadiabatic effects.
P. Gamallo, C. Petrongolo, M. Paniagua, M. González.

Photodissociation quantum dynamics of diatomic molecules in a quantum solvent (^4He nanodroplets)
A. Vilà, M. González, R. Mayol

Oxidation of atmospheric mercury by the OH radical. Ab initio and quasiclassical trajectory study
M. Paniagua, R. Martínez, M. González

8th international meeting on photodynamics and related aspects (Photodynamics)
Oaxaca (Mexico)

Adiabatic and nonadiabatic dynamics of $CH(X^2P) + H(^2S)$ and deuterated reactions.
C. Petrongolo, P. Gamallo, P. Defazio, S. Akpinar.

II Reunión de jóvenes investigadores en coloides e interfases (JICI-II).
Granada (Spain)

Efecto del crowding macromolecular en reacciones enzimáticas
C. Balcells, I. Pastor, L. Pitulice, E. Vilaseca, S. Madurga, A. Isvoran, M. Cascante, F. Mas

Master Química X
Barcelona (Spain)

Efecte del crowding macromolecular en reaccions enzimàtiques
C. Balcells, I. Pastor, E. Vilaseca, S. Madurga, M. Cascante, F. Mas

XXX Reunió de la xarxa de Referència en Química Teòrica i Computacional de Catalunys (XrQTC)
Barcelona (Spain)

Enzyme size as a modulator of macromolecular crowding effect in enzyme kinetics
I. Pastor, M. Via, C. Balcells, S. Madurga, E. Vilaseca, M. Cascante, F. Mas

Simple chemical reactions in ^{4}He nanodroplets
M. González, R. Mayol, A. Vilà

Nitrile compounds in Titan's atmosphere
J.M. Lucas, A. Aguilar, D. Ascenzi, J.M. Bofill and E. López

Quantitative study of the eigenstates of a Hydrogen molecule confined inside Single Walled Carbon Nanotubes
M. Mondelo-Martell, F. Huarte-Larrañaga

VIII Congreso de la Federación Española de Biotecnólogos/Biotech Annual Congress 2014 (BAC-2014)
Barcelona (Spain)

The effect of enzyme size as a modulator of macromolecular crowding effect in enzyme kinetics
C. Balcells, I. Pastor, E. Vilaseca, S. Madurga, M. Cascante, F. Mas

Frontiers in Surface and Materials Science: Theory and Practice
Barcelona (Spain)

Enzyme size as a modulator of macromolecular crowding in enzyme kinetics
I. Pastor, M. Via, C. Balcells, S. Madurga, E. Vilaseca, M. Cascante, F. Mas

Emergent Colloidal Dynamics Far From Equilibrium
Lausanne (Switzerland)

Molecular dynamic study of thin film rupture due to external electric field
M. Nedyalkova, S. Madurga, N. Panchev, S. Pisov

Deustche Physikalische Gesellschaft - DPG Spring Meeting
Technische Universität Dresden, Dresden (Germany)

Cost-Effective Catalysis on Early Transition Metal Carbides Surfaces
F. Viñes

International Congress of Theoretical Aspects in Catalysis - ICTAC15
University College London, London (UK)

Cost-Effective Catalysis on Transition Metal Carbides Surfaces
F. Viñes

3rd General Meeting of the European COST Action CM1104
Universitat de Barcelona, Barcelona (Spain)

Chairman
K.M. Neyman

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

Theoretical study of the CO interactions with mononuclear platinum species supported on nanoparticulate ceria
H.A. Aleksandrov, K.M. Neyman, G.N. Vayssilov

Atomically dispersed M species (M = Pd, Ni, Cu) in ceria nanoparticles: Stability and red-ox processes
A. Figueroba, K.M. Neyman

Origin, stability, and effect of atomically dispersed Pt on nanostructured catalytic Pt-CeO2 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

I Encuentro de Jóvenes Investigadores de la SECAT
Universitat de Málaga, Málaga (Spain)

Superficies de Carburo de Molibdeno: Activación y Ruptura de la Molécula de CO_2
S. Posada-Pérez, F. Viñes, P.J. Ramirez, A.B. Vidal, J.A. Rodriguez, F. Illas

Physics@FOM Conference
FOM, Veldhoven (The Netherlands)

Theoretical study of the high spin-low spin relaxation in iron based spin crossover compounds: beyond single mode approximation
A. Rudavskyi, G. Lof, C. Sousa, J. Tatchen, C. Marian, C. de Graaf, R. Broer

VII European Workshop on Molecular Magnetism- Jujols VII
Max Planck Institute for Chemical Energy Conversion, Mülheim an der Ruhr (Germany)

Temperature dependent high spin - low spin relaxation on spin crossover materials
A. Rudavskyi, C. Sousa, C. de Graaf, R. Broer

The Triplet-Singlet Gap in the m-Xylylene Radical: A Not So Simple One
D. Reta-Mañeru

Remarks on the exact energy functional for fermions: a wave-function theories using the Löwdin partitioning technique
I.d.P.R. Moreira

American Chemical Society National Meeting, Physical Chemistry Division
American Chemical Society, Texas (USA)

Analysis of the spin-crossover mechanism in Fe(II) complexes
R. Broer, M. Etinski, C. de Graaf, R.W.A. Havenith, C. Marian, A. Rudavskyi, C. Sousa, J. Tatchen

Theoretical Studies of Au/TiC and Cu/TiC based catalysts for CO_2 activation and hydrogenation
F. Illas, J.A. Rodriguez

Promoting Female Excellence in Theoretical and Computational Chemistry II
University of Tromsø, Oslo (Norway)

Analysis of the spin-crossover mechanism in Fe(II)
R. Broer, M. Etinski, C. De Graaf, R.W.A. Havenith, C.M. Marian, A. Rudavskyi, C. Sousa, J. Tatchen

11th International Conference on Relativistic Effects in Heavy-Element Chemistry and Physics
Comenius University, Smolenice Castle (Czech Republic)

Mechanisms of spin crossover in Fe(II) complexes
A. Rudavskyi, R. Broer, M. Etinski, C. de Graaf, R.W.A. Havenith, C.M. Marian, C. Sousa, J. Tatchen

10th Congress of the World Association of Theoretical and Computational Chemists, WATOC 2014
Pontificia Universidad Católica de Chile, Santiago de Chile (Chile)

Spin Crossover in Fe(II) Metal-Organic Complexes
A. Rudavskyi, R. Broer, M. Etinski, C. de Graaf, R.W.A. Havenith, C.M. Marian, C. Sousa, J. Tatchen

Analyzing the electronic structure of molecules using Continuous Symmetry Measures
P. Alemany

Solvatochromic effects on a D-π-A type organic dye with a quinoidal thiophene π-bridge
C. Climent, D. Casanova, P. Alemany

Advances in Computational Spectroscopy 2014, COST CODECS
Matej Bel University, Bratislava (Slovakia)

Absorption Spectrum of $[Fe(bpy)_3]^{2+}$: Beyond the Static Approach
A. Domingo, C. Sousa, C. de Graaf

XI Simposio de Investigadores Jóvenes RSEQ-Sigma Aldrich
Universidad del País Vasco, Bilbao (Spain)

Synthesis and Study of an Organic Molecule with Paramagnetic Response
D. Reta-Mañeru, C. Heras, I.d.P.R. Moreira, J.M. Bofill, A. López-Calahorra

50th Syposium on Theoretical Chemistry 2014 (STC2014)
Universität Wien, Vienna (Austria)

Remarks on the exact energy functional for fermions: a wave-function theories using the Löwdin partitioning technique
I.d.P.R. Moreira, M. Caballero, J.M. Bofill

Locating Saddle Points of any Index on Potential Energy Surfaces by the Generalized Gentlest Asecnt Dynamics
J. M. Bofill, W. Quapp

RCTF2014 14ème Recontre des Chimistes Théoriciens Francophones
Université Pierre et Marie Curie, Paris (France)

Towards theoretical modeling of realistic systems in heterogeneous catalysis form first principles
F. Illas

XL Congreso Internacional de Químicos Teóricos de Expresión Latina - QUITEL
Universidad San Francisco de Quito, Galápagos (Ecuador)

New Catalysts for CO_2 activation and hydrogenation based on Au/TiC and Cu/TiC: Theoretical modeling and experiments
F. Illas

DFG-out kinase inhibitors: Understanding their binding mechanism
L. Coronel, E. Yurci, J. Mayans, J.M. Granadino-Roldan, M.S. Tomás, M.D. Pujol, J. Rubio-Martínez

Steered molecular dynamics and umbrella sampling approaches to the binding mechanism of DFG-out p38α kinase inhibitors
J. Clark, J.M. Granadino-Roldán, M.S. Tomás, M.D. Pujol, J. Rubio-Martínez

XXV Congresso Nazionale Della Societa Chimica Italiana (SCI)
Università della Calabria, Cozenza (Italia)

First principles modeling of realistic systems in heterogenous catalysis
F. Illas

Symposium on clusters, Cluster Assemblies and Nano-scale Materials - III
Harish-Chandra Research Institute, Allahabad (India)

Ionicity, Covalency and the Cluster-to-Bulk Transition in Nano-Oxides
S. T. Bromley

European Materials Research Society (EMRS) – Fall Meeting 2014, Symposium D: Transparent Conducting Oxides and Related Materials
Warsaw University of Technology, Warsaw (Poland)

Bandgap Engineering via Nanoporosity
S. T. Bromley

Cosmic Dust VII
Osaka Sangyo University, Osaka (Japan)

A Bottom-up Computational Modelling Approach to the Formation and Properties Silicate Dust
S. T. Bromley

COST Action CM1104 meeting - Reducible oxide chemistry, structure and functions
Zaragoza Scientific Center for Advanced Modeling (ZCAM), Zaragoza (Spain)

Approaching the nanocluster-to-bulk structural transition in CeO_2, TiO_2 and SiO_2
S. T. Bromley

Symposium on Clusters, Nanoparticles and Nanostructures in Catalysis and Beyond
Universitat de Barcelona, Barcelona (Spain)

Organizing Committee
K.M. Neyman

From supported oxide nanoclusters to nanoporous oxide polymorphs
S. T. Bromley

Studies of nanostructuring effects on model catalysts
S.M. Kozlov, K.M. Neyman

SFB "Functional Oxide Surfaces and Interfaces"
Institute of Materials Chemistry, Vienna University of Technology, Vienna (Austria)

Towards more realistic density functional modelling of nanostructures relevant to heterogeneous catalysis
K.M. Neyman

International Conference "Molecular Complexity in Modern Chemistry"
Moscow (Russia)

Towards realistic first-principles modelling of complexity in heterogeneous catalysis
K.M. Neyman

XI Girona Seminar on Carbon, Metal, and Carbon-Metal Clusters: From Theory to Applications
Girona (Spain)

First-principles studies of metal particles in catalysis
K.M. Neyman

CIC energiGUNE
Parque Tecnológico de Álava, Miñano (Spain)

First-principles modelling of complex nanostructures: From catalysis to energy technologies
K.M. Neyman

247th National Meeting of the American Chemical Society, Symposium "Clusters in Catalysis"
Dallas (USA)

Density-functional studies in heterogeneous catalysis: Extended surfaces or nanoparticles?
K.M. Neyman

248th National Meeting of the American Chemical Society
San Francisco (USA)

CO adsorption on mononuclear platinum species supported on nanoparticulate ceria
H.A. Aleksandrov, K.M. Neyman, G.N. Vayssilov

Clusters 2014: Workshop on reactivity and catalysis of metallic nanoclusters
Esbo (Finnland)

Density-functional modelling of metal nanoparticles relevant for catalysis
K.M. Neyman

Theoretical investigations of metal particles as potential PEMFC electrocatalysts
P. Jennings, R.L. Johnston, H.A. Aleksandrov, K.M. Neyman

VI Conference in Education and Modeling in Basic Sciences
Universidad de Medellín, Medellín (Colombia)

Modelling the effect of metal-support interactions in nanostructured heterogeneous catalysts based on Pt and CeO_2
A. Bruix, K.M. Neyman, F. Illas

WG3 Meeting of the COST Action CM1104 "Reducible oxide chemistry, structure and functions"
Charles University in Prague (Czech Republic)

Progress in modelling of ionic metal species in CeO2-based catalytic nanomaterials
K.M. Neyman, A. Bruix, A. Figueroba, F. Illas, J. Libuda, V. Matolin*Relative stability of*

mononuclear platinum species supported on nanoparticulate ceria and adsorption of CO on them
H.A. Aleksandrov, K.M. Neyman, G.N. Vayssilov
Substrate effects on Pt nanoparticles. Electronic and structural differences induced by CeO_2(111) and MgO(100) on ~1 nm Pt clusters
S.M. Kozlov, K.M. Neyman, S. Fabris

4th International Symposium of Intermetallic Compounds in Catalysis
Santa Margherita de Ligure (Italy)

Geometric and electronic structure of Pd-based intermetallic nanoparticles
S.M. Kozlov, K.M. Neyman

General Meeting of COST-MP0903 Action "Nanoalloys as Advanced Materials"
Santa Margherita de Ligure (Italy)

Modeling of bimetallic and intermetallic nanoparticles containing Pd
S.M. Kozlov, K.M. Neyman

Evaluation Meeting of COST-MP0903 Action "Nanoalloys as Advanced Materials" (April 9)
Santa Margherita de Ligure (Italy)

Report on the activities of the Working Group 3 "Catalysis"
K.M. Neyman

4th Workshop Quantum Days in Bilbao
Centro Vasco de Matemáticas Aplicadas, Bilbao (Spain)

Quantum reaction dynamics in gas phase and in a quantum solvent (^{4}He nanodroplets)
M. González, A. Vilà, R. Mayol, P. Gamallo, M. Paniagua, C. Petrongolo

Helium-mediated Synthesis, Soft-landing and Spectroscopy of Metal Nanoparticles on Surfaces (HeSSSMe 2014)
Consejo Superior de Investigaciones Científicas, Madrid (Spain)

Molecular photodissociation processes in helium nanodroplets. A theoretical quantum dynamics approach
A. Vilà, M. González, R. Mayol

II Jornada de Bioinformàtica i Biologia Computacional
Barcelona (Spain)

Development of new drugs against tuberculosis. Computer-aided identification of inhibitors of the enzyme CDP-methylerythritol synthase
C. Obiol-Pardo, C. García Sabaté, E. Schreiber, J. Rubio-Martínez. S. Imperial

14th Fock meeting of Quantum and Computational Chemistry
Samara (Russia)

Continuous Shape and Symmetry Measures: a useful tool in structural chemistry
P. Alemany

Optical properties of 4-bromobenzaldehyde derivatives in chloroform solution
C. Climent, D. Casanova, P. Alemany

6th Time-Dependent Density-Functional Theory: Prospects and Applications.
Benasque (Spain)

Non-Adiabatic Dynamics with Conditional Wave Functions
G. Albareda

78. Jahrestagung der Deutsche Physikalische Gesellschaft und DPG-Frühjahrstagung.
Berlin (Germany)

Non-Adiabatic Molecular Dynamics with Conditional Wave Functions
G. Albareda, H. Appel, I. Franco, A. Abedi, Á. Rubio

CECAM Workshop. Recent progress in adiabatic and non-adiabatic methods in quantum dynamics.
Lausanne (Switzerland)

A Correlated Electron-Nuclear Dynamics with Conditional Wave Functions
G. Albareda, H. Appel, I. Franco, A. Abedi, Á. Rubio

Jornada d'Investigadors Predoctorals Interdisciplinària (2nd JIPI)
Universitat de Barcelona, Barcelona (Spain)

Astrochemistry & Nitrile compounds
E. López

4th Workshop on High Dimensional Quantum Dynamics: Challenges and Opportunities
Université de Strasbourg, Mittelwihr (France)

MCTDH Study of the eigenstates of a H_2 molecule confined inside a SWCNT
F. Huarte-Larrañaga, M. Mondelo-Martell

SPECMO 2014 : "New experimental and theoretical developments in molecular spectroscopy : pushing the limits"
Université Franco-Allemande, CNRS, Corsica (France)

Quantum Dynamics study of the eigenvalue spectrum of a Hydrogen molecule confined inside a Single Walled Carbon Nanotube
M. Mondelo-Martell, F. Huarte-Larrañaga

XI Carbohydrate symposium
Universitat de Logroño, Logroño (Spain)

Molecular mechanisms of retaining glycosyltransferases. QM/MM metadynamics investigations
C. Rovira

Minisymposium on structural biology
University of Oslo, Oslo (Sweden)

The catalytic mechanism of catalase-peroxidases (KatGs)
C. Rovira

International workshop on Biomembranes: from fundamentals to applicationss
CSC – IT Center for Science, Espoo, Helsinki (Finnland)

The effects of chloroform in bilayer interleaflet coupling
R. Reigada

RESEARCH STAYS IN RECOGNIZED CENTERS

M. Albertí — **Univeristà di Perugia, Dipartimento di Chimica (Italy)**
Professor on sabbatical. January-July 2014

D. Reta-Mañeru — **Indian Institute of Technology Bombay, Mumbai (India)**
Predoctoral research stay. January-Feburary 2014

J. Ribas — **Japan Atomic Energy Agency, Center for Computational Science and E-systems (Japan)**
Invited visiting scientist. January 2014

M. Fumanal — **Trinity College Dublin, Computational Spintronics Group (Ireland)**
Predoctoral research stay. April-May 2014

S.M. Kozlov — **Scuola Internazionale Superiore di Studi Avanzati, Trieste (Italy)**
Predoctoral research stay. March-May 2014

P. Gamallo — **MATGAS, Barcelona (Spain)**
Invited visiting professor. May-July 2014

X. Giménez — **MATGAS, Barcelona (Spain)**
Invited visiting professor. May-July 2014

P. Alemany — **Donostia International Physics Center, Donostia (Spain)**
Invited visiting scientist. June 2014

C. Sousa — **Universitat de Groningen, Groningen (The Netherlands)**
Invited visiting professor. July 2014

C. Climent — **Donostia International Physics Center, Donostia (Spain)**
Predoctoral research stay. July 2014

K.M. Neyman	**Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen (Germany)** Invited visiting scientist. July-August 2014
A. Falceto	**Cornell University, Department of Chemistry and Chemical Biology (USA)** Predoctoral research stay. July-October 2014
D. Reta-Mañeru	**University of Strasbourg, Strasbourg (France)** Predoctoral research stay. September-November 2014
P. Alemany	**Departamento de Química, Universidad Católica del Norte, Antofagasta (Chile)** Invited visiting scientist. October 2014
M. Llunell	**Donostia International Physics Center, Donostia (Spain)** Research stay. November 2014

PARTICIPATION IN COMPETITIVE FUNDED RESEARCH PROJECTS

Grup d'Estructura Electrònica.
Santiago Alvarez Reverter, Universitat de Barcelona
2009SGR1459, 2012-2014
Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR)

Grup d'Estructura Electrònica.
Santiago Alvarez Reverter, Universitat de Barcelona
2014SGR662, 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 Bioquímica Integrativa
Marta Cascante Serratosa, Universitat de Barcelona
2014SGR1017, 2014-2016
Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR)

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)

Laboratori de Ciència de Materials Computacional
Francesc Illas Riera, Universitat de Barcelona
2014SGR97, 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)

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)

Estructura electrónica y propiedades de moléculas y sólidos inorgánicos.
Eliseo Ruiz Sabin and Pere Alemany Cahner, Universitat de Barcelona
CTQ2011-23862-C02, 2009-2014
Dirección General de Investigación

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, 2012-2014
Dirección General de Investigación (DGI)

Dinámica de procesos químicos mediante haces moleculares y métodos teóricos.
Antonio Aguilar Navarro (IP1), Universitat de Barcelona
CTQ2010-16709, **2011-2014**
Ministerio de Ciencia e Innovación (MICIIN)

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)

Estructura y dinámica de reacciones químicas, mediante modelos extendidos de camino de reacción y la teoría de la función de onda.
Josep Maria Bofill Villà, Universitat de Barcelona
CTQ2011-22505, 2012-2014
Dirección General de Investigación (DGI)

Propiedades magnéticas y transformaciones de fase en cristales con propiedades de interés tecnológico.
Juan J. Novoa Vide, Universitat de Barcelona
MAT2011-25972.2012, 2012-2014
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)

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 reacciones de oxidación iniciadas por HO, O3 y NO3
Josep Maria Anglada Rull, CSIC
CTQ2011-27812, 2012-2014
Dirección General de Investigación y Gestión del Plan nacional de I+D+I (MICINN)

Simulation of reactive processes in heme enzymes, glycoside hydrolases/transferases and peptide-bound nanoparticles by means of ab initio molecular dynamics-based methods
Carme Rovira Virgili, Universitat de Barcelona
CTQ2011-25871, 2012-2014
Ministerio de Economia y Competitividad (MINECO)

Diseño asistido por ordenador y síntesis de nuevos inhibidores enzimáticos de naturaleza heterocíclica con potencial actividad antitumoral.
Jaime Rubio Martínez . Universidad de Barcelona.
CTQ2011-29285-C02-02 , 2012-2014
Ministerio de Ciencia e Innovación. Proyectos de Investigación fundamental no orientada.

Estructura, Redes y Motivos Celulares.
Ramon Reigada Sanz, Universitat de Barcelona
BFU2010-21847-C02-0 (subprograma BMC), 2011-2013 (Extended until 2014)
Ministerio de Ciencia e Innovación (MICINN)

Modelizacion de materiales formados por mezclas de oxidos con relevancia tecnologica y medioambiental
Stefan Bromley, Universitat de Barcelona
MAT2012-30924, 2013-2015
Ministerio de Economía y Competitividad (MINECO)

India-Spain bilateral Project on Theoretical and computational investigation of molecular magnets and extended systems as candidates of exotic nanomaterials with useful properties
Francesc Illas Riera, Universitat de Barcelona
PRI-PIBIN-2011-1028, 2012-2014
Ministerio de Economía y Competitividad

Knowledge led structure prediction for nanostructures
Scott Woodley, University College London
EP/K038958/1, 2013-2018
Engineering and Physical Science Research Council (EPSRC), United Kingdom

Theoretical Chemistry and Computational Modelling
Manuel Yáñez, Universidad Autónoma de Madrid
***TCCM-EJD**, 2014-2018*
Horizon 2020 – Research and Innovation Framework Programme

Planetary entry integrated models (Phys4Entry).
Ramón Sayós Ortega, Universitat de Barcelona
Referencia, FP7-SPACE-2009-1, 242311
7th Framework Programme of the European Union

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'

Metabolic Flux Analysis and Cancer (METAFLUX)
Jaime Rubio Martínez . Marta Cascante Serratosa. Universitat de Barcelona.
PITN-GA-2010-264780, 2010-2014
FP7-PEOPLE. European Commission.

Reducible oxide chemistry, structure and functions
Francesc Illas Riera, (representant d'Espanya), Konstantin Neyman (representant adjunt), Universitat de Barcelona
CM1104, 2012-2016
European Framework for Cooperation in Science and Technology (COST)

Explicit Control Over Spin-states in Technology and Biochemistry (ECOSTBio)
Marcel Swart, Universitat de Girona, Carme Sousa, Universitat de Barcelona
CM1305, 2013-2017
European Framework for Cooperation in Science and Technology (COST)

Network for intermetallic compounds as catalysts for steam reforming of methanol
Konstantin Neyman, Universitat de Barcelona (Spanish representative in the Management Committee)
CM0904, 2010-2014
European Framework for Cooperation in Science and Technology (COST)

Nanoalloys as advanced materials: from structure to properties and applications
Konstantin Neyman, Universitat de Barcelona (Spanish representative in the Management Committee; lider of the Workgroup "Catalysis")
MP0903, 2010-2014
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)

Reducible oxide chemistry, structure and functions
Konstantin Neyman, Universitat de Barcelona (deputy Spanish representative in the Management Committee)
CM1104, 2012-2016
European Framework for Cooperation in Science and Technology (COST)

Device simulation (RF), NannoMechanics and Spintronics Entidad financiadora: Graphene Flagship.
David Jiménez Jiménez, Universitat Autónoma de Barcelona
604391 Graphene Flagship, 2013-2016
FET. European Union

Dynamical processes in open quantum systems: pushing the frontiers of theoretical spectroscopy.
Ángel Rubio Secades, Universidad del País Vasco and Fritz Haber Institute of the Max Planck Society
ERCDYNAMO, 2011-2016
European Research Council. Advanced Grant.

Simulación de sistemas cuánticos nanostructurados fuera del equilibrio.
Ángel Rubio Secades, Universidad del País Vasco
IT578-13, 2013-2018
Grupos Consolidados. Gobierno del País Vasco.

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

Premi ICREA Academia
E. Ruiz, Universitat de Barcelona
2014-2018
Institució Catalana de Recerca i Estudis Avançats (ICREA)

Institut de Química Teòrica
i Computacional