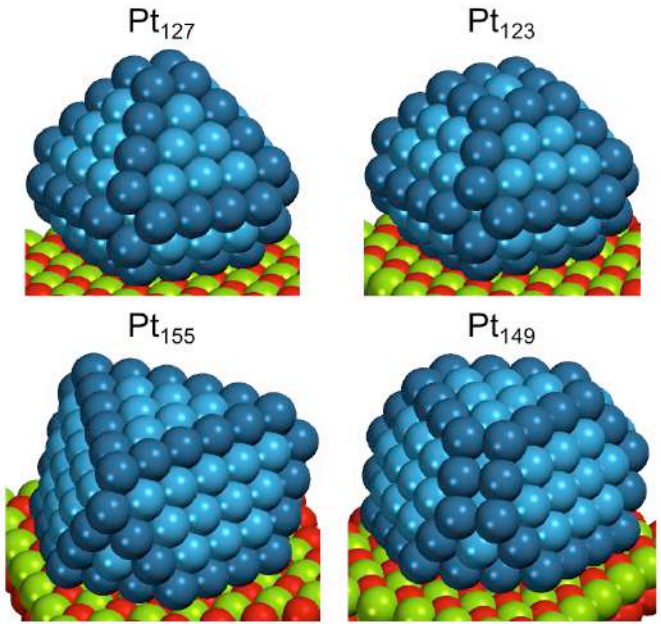
Institut de Química Teòrica i Computacional

UNIVERSITAT DE BARCELONA

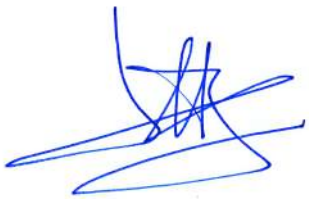
Institut de Química Teòrica i Computacional de la Universitat de Barcelona (IQTCUB)



Activity Report 2013

The Institute of Theoretical and Computational Chemistry of the *Universitat de Barcelona* (IQTCUB) is one of the research institutes of this university; it was created by the university Government Board on November 27th and involves professors and researchers of differents departments of the Faculties of Chemistry and Physics of the *Universitat de Barcelona*. The common theme of the research projects conducted at the Institute is the use of methods that are rooted in quantum chemistry and/or solid-state physics, together with methods stemming from computational chemistry or physics. Although research at IQTCUB is mainly focused on chemistry, it is different from one would expect of a traditional chemist. Indeed, the tools employed by the researchers at IQTCUB do not belong to a typical laboratory, but to a virtual computational "laboratory". This "laboratory" is usually a gateway to a supercomputing center with hundreds or thousands of processors, such as Marenostrum, at the *Barcelona Supercomputing Center*, or the supercomputers of the *Centre de Supercomputació de Catalunya* (CESCA), which are used by many researchers at IQTCUB almost on a daily basis. The main objective of theoretical and computational chemistry is to achieve a detailed understanding of chemical processes in order to assist in the interpretation of experimental results and to make predictions that should lead to new experiments. In so doing, this discipline can provide new concepts that can pave the way to the rational design of new materials with tailored properties, to the discovery of new drugs, to new reactions that furnish important products with better efficiency and selectivity, to an improvement of chemical processes to make them more efficient and more environmentally friendly and to propose new sustainable sources of energy, thereby tackling challenges that our society is currently facing. It is clear that these goals are also shared with other disciplines; it is precisely such interdisciplinarity what makes the theoretical insight so relevant.

In the past few years, we have been experiencing a harsh economical situation. Yet the Research Vicerector has kept supporting the Institute. This continuous support has been invaluable and we would like to fully acknowledge it. Thanks to this support, we have been able to maintain and even improve a computational infrastructure where IQTCUB professors and researchers carry out high quality competitive scientific research. The following activity report shows the full vitality of our Institute. The remarkable scientific productivity of IQTCUB members in research lines as different as drug design, heterogeneous catalysis, nanostructures, and atmospheric chemistry clearly demonstrates the growing impact of our research. 2013 marks an end of a cycle since my first tenure as Director of the Institute has come to an end. In the years to come we do hope that we will show that our project continues to deserve the full support of the University. We also hope that we will maintain the high scientific standards thus far achieved, as evidenced by the external evaluation that can be read in our 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. Pere Alemany Cahner	*Secretary*
Prof. Ramón Sayós Ortega	*Treasurer*
Prof. Fermín Huarte Larrañaga	*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 his 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 Biochemisry and soft matter**

Using the battery 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 77 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
Garcia Bach	Maria Àngels	Fundamental Physics
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
Madurga Díez	Sergio	Physical Chemistry
Reigada Sanz	Ramón	Physical Chemistry

Other categories (Professors Associats)

Gamallo Belmonte	Pablo	Physical Chemistry
Tercero Mohedano	Javier	Inorganic Chemistry

ICREA Research Professors ICREA

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

Postdoctoral contracts

Juan de la Cierva contract

Pastor del Campo	Isabel	Physical Chemistry
Viñes Solana	Francesc	Physical Chemistry
Jover Modrego	Jesús	Inorganic Chemistry

Ramón y Cajal contract

Casanova Casas	David	Physical Chemistry
Ribas Ariño	Jordi	Physical Chemistry

Other

Álvarez Falcón	Leny	Physical Chemistry
Dos Santos Politi	Jose Roberto	Physical Chemistry
Kovács	Gábor	Physical Chemistry
Tosoni	Sergio	Physical Chemistry

Ph D students

FPI (Associated with Ministerio Research Grants)

Aguilar Fargas	Javier	Physical Chemistry
Alonso Gil	Santiago	Organic Chemistry
Bruix Fusté	Albert	Physical Chemistry
Caballero Puig	Marc	Physical Chemistry
Carreras Conill	Abel	Physical Chemistry
Climent Biescas	Clàudia	Physical Chemistry
Falceto Palacín	Andrés	Inorganic Chemistry
Jurado Sáez	Manuel	Physical Chemistry

Vela Llausi	Sergi	Physical Chemistry
Vilà Casanova	Arnau	Physical Chemistry

FPU (Spanish Ministerio Program)

Capdevila Cortada	Marçal	Physical Chemistry
Gómez Coca	Silvia	Inorganic Chemistry
Kozlov	Sergey M.	Physical Chemistry
Rojas Cervellera	Victor	Organic Chemistry

UB own program

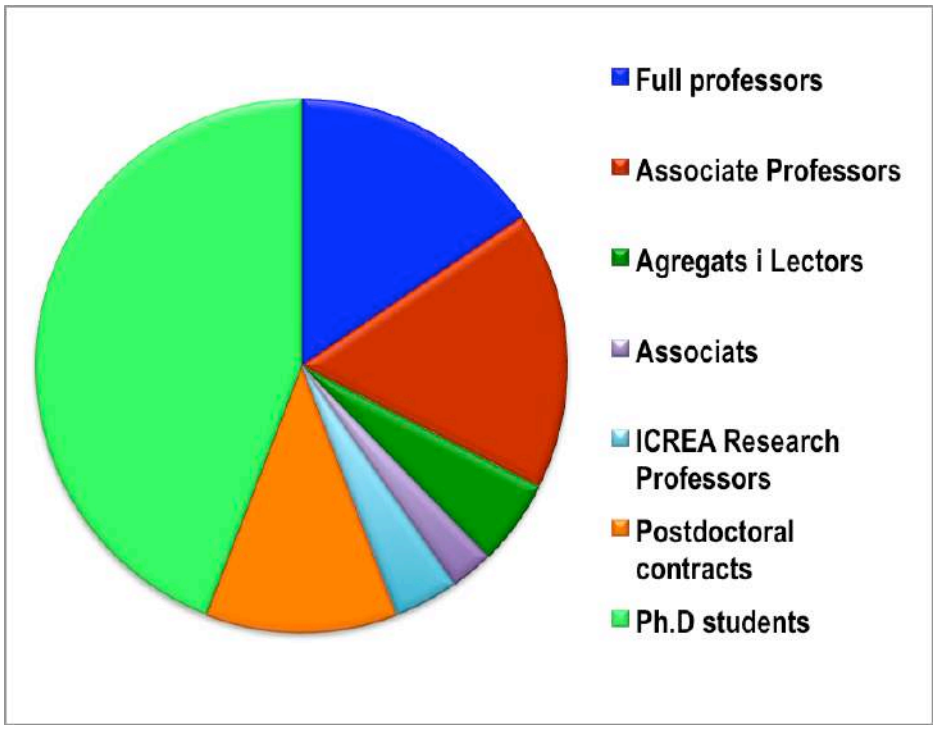
Fumanal Quintana	Maria	Physical Chemistry
Lamiel Garcia	J. Oriol	Physical Chemistry

FI (Catalan Government Program)

López Marne	Estefanía	Physical Chemistry

Other funding

Aravena Ponce	Daniel	Inorganic Chemistry
Balcells Nadal	Cristina	Physical Chemistry
Cremades Martí	Eduard	Inorganic Chemistry
Conejeros Espíndola	Sergio	Physical Chemistry
Demiroglu	Ilker	Physical Chemistry
Figueroba Sánchez	Alberto	Physical Chemistry
Iglesias Fernández	Javier	Organic Chemistry
Maxwell	Lindley	Inorganic Chemistry
Mondelo Martell	Manel	Physical Chemistry
Morales Martínez	Roser	Inorganic Chemistry
Peigné	Benjamin	Inorganic Chemistry
Prats Garcia	Hèctor	Physical Chemistry
Raich Armendáriz	Lluís	Organic Chemistry
Rafels Ybern	Albert	Physical Chemistry
Reta Mañeru	Daniel	Physical Chemistry
Ruiz Martínez	Antonio	Inorganic Chemistry
Ruiz Puigdollers	Antonio	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.

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 300.000 €)

Machine type HP Cluster
Operating System SLES11
Services Calculation cluster
Structure 23 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: 2 gigabit network card (calculation network) + 1 IPMI card (OOB)

GPU cluster (approximate value 20.000 €)

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)

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)

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

Node ASUS ESC4000 G2
CPU: 2x2GHz Xeon SixCore
RAM: 24GB
HD: 1x2TB hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (OOB)

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 .....2788 CPUs

Memory .....18616 GB RAM

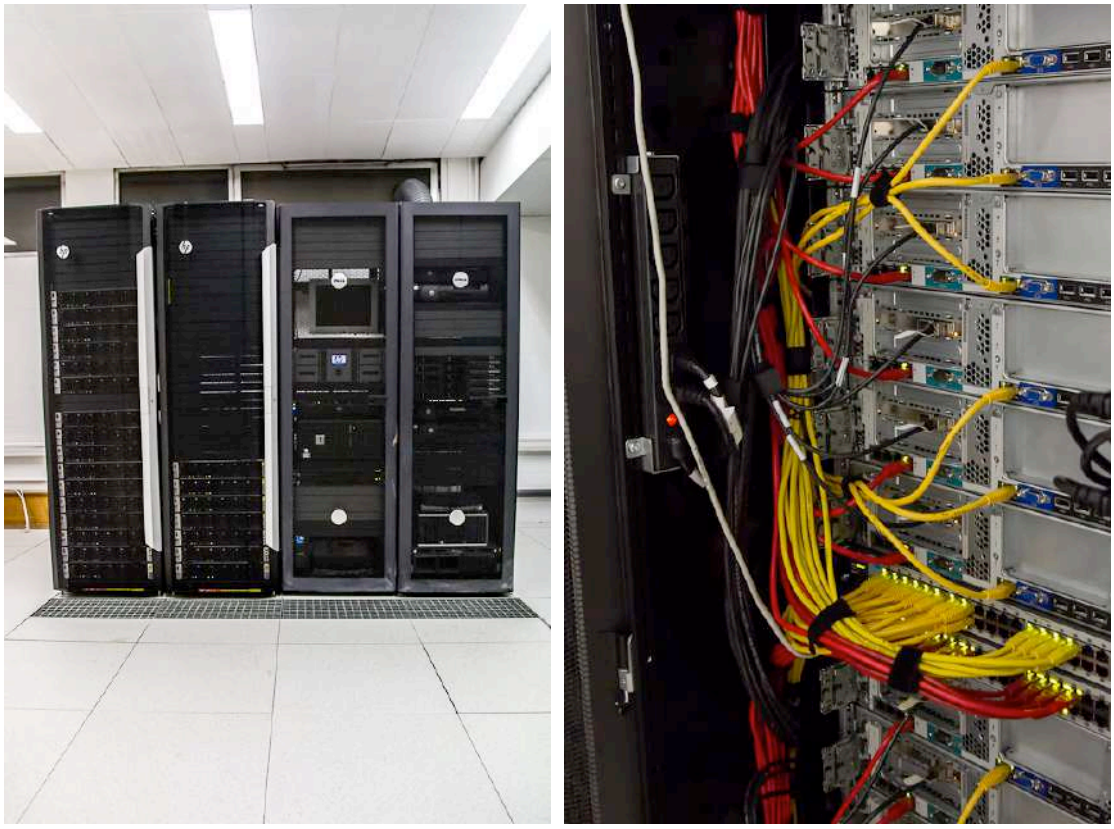
Calculation disk capacity ..... 170 TB

Data user disk capacity ..... 32 TB

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

2.000.000 €*

*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 2013 is provided.

a. *4th IQTCUB workshop*. This one-day workshop aimed at the dissemination of the research done at the IQTCUB took place on June 21st, 2013. The IQTCUB members and some internationally acknowledged speakers present the most recent work. This year we highlight the participation of Prof. Piero Ugliengo from the *Università di Torino,* Dr. Emilio Martínez Núñez from *Universidad de Santiago de Compostela* and Dr. Ramón Crehuet Simon from *Institut de Química Avançada, CSIC*. The IQTCUB assigned a budget to cover the traveling expenses Prof. Ugliengo and Dr. Martínez as well as the cattering service offered to all assistants. Total cost: 1721 €

b. Promotion and encouragement of research. This year the IQTCUB has offered a total of four 2000 € grants aimed to help students to initiate a scientific careers. These grants 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 grants have been awarded to Mrs. Hector Prats, Antonio Ruíz, Miquel Blancafort, and Ms. Cristina Balcells. Total cost: 8000 €

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 2013 edition has been the third one and has been very successful with over 30 students requesting to participate. The course took place during June 25-28th 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, 1st-5th with an attendance of 25 students. IQTCUB has covered catering expenses with a total cost of 236 €.

Picture corresponding to the “Advanced Course in Computational Chemistry” that took place in July 2013 at the Chemistry Faculty of the *Universitat de Barcelona*.

II.2 IQTCUB SEMINARS AND CONFERENCES

Fourteen seminars have been organized by IQTCUB during 2013.

1. **Prof. Henrik Ottoson** (Uppsala University) Sweden

   Excited State Aromaticity and Antiaromaticity: Opportunities for Photophysical and Photochemical Rationalizations

   January 16th, 2013

2. **Dra. Anapaola Migani** (Centre d'Investigacio en Nanociencia i Nanotecnolgia, CIN2) Spain

   Advanced Modeling of Hole and Acceptor States for Methanol on TiO_2

   February 20th, 2013

3. **Mrs. Miroslava Nedyalkova** (University of Sofia) Bulgaria

   Molecular dynamics simulation of the spherical electrical double layer of a soft nanoparticle: Effect of the surface charge and counterion valence

   March 1st, 2013

4. **Prof. José Valderrama** (Universidad de la Serena) Chile

   Correlation and Prediction of the Physical and Physicochemical Properties of Ionic Liquids

   May 9th, 2013

5. **Prof. Natia Frank** (University of Victoria) Canada (MAGISTER conference)

   Open-Shell Organic Electronic Materials

   May 28th, 2013

6. **Prof. Ponnadurai Ramasami** (University of Mauritius) Mauritius

   Computational Chemistry at the Univeristy of Mauritius: Past, Present & Future

   June 4th, 2013

7. **Prof. Joan Bertran** (Universitat Autònoma de Barcelona) Spain (MAGISTER conference)

   From free energy surfaces to an insight in enzymatic catalysis

   June 27th, 2013

8. **Dr. Albert Rimola** (Universitat Autònoma de Barcelona) Spain

   Computational modelling of gas-grain chemical processes in the interstellar medium

   July 17th, 2013

9. **Dr. Juan M. Randazzo** (Consejo Nacional de Investigaciones Científicas y Técnicas, CONICET) Argentina

   Reactive dynamics and bound states study of the Li+ + H + H system in the Born-Oppenheimer approximation.

   October 11th, 2013

10. **Prof. Sambhu Datta** (Indian Institute of Technology Bombay) India

    Theoretical Investigation of Magnetic and Conducting Properties of Substituted Silicon Chains: Hydrogen and Oxo-Verdazyl Ligands.

    October 28th, 2013

11. **Prof. Michael Probst** (Universität Innsbruck) Austria

    Some aspects of computational material science with respect to the ITER reactor

    November 4th, 2013

12. **Dr. Santiago Schnell** (University of Michigan Medical School) USA

    Designing Simulations to Investigate Reactions Inside Cells

    November 12th, 2013

13. **Prof. Jean Paul Malrieu** (Université Paul Sabatier) France

    Magnetism of polycyclic conjugated hydrocarbons and graphene

    November 15th, 2013

14. **Prof. John Plane** (Head of School of Chemistry, University of Leeds) United Kingdom

    Meteoric Smoke in the Earth's Upper Atmosphere

    November 21st, 2013

II.3 IQTCUB INVITED RESEARCHERS

During 2013, a total of sixteen researchers from all over the world have spent some time at the IQTCUB collaborating in different research projects.

1. **Dr. Juan Martín Randazzo** (invited visitor)
   Centro Atómico de Bariloche, Argentina
   January-December, 2013

2. **Patanachai Janthon** (invited visitor)
   Kasetsart University, Bangkok, Thailand
   January-May, 2013

3. **Ichraf Oueslati** (ITN visitor)
   Observatoire de Paris – Meudon, Paris, France
   April-May and December, 2013

4. **Julian Gebhardt** (invited visitor)
   Friedrich-Alexander Universität Erlangen-Nürnberg, Germany
   April-July, 2013

5. **Anderson dos Reis Albuquerque** (invited visitor)
   São Paulo University, Brazil
   April-October, 2013

6. **Miroslava Nedyalkova** (invited visitor)
   University of Sofia, Bulgaria
   June-July, 2013

7. **Prof. Maria Marta Branda** (invited visitor)
   Universidad Nacional del Sur, Argentina
   July, 2013

8. **Prof. Georgi N. Vayssilov** (invited visitor)

University of Sofia, Bulgaria
July, 2013

9. **Dr. Hristiyan A. Aleksandrov** (invited visitor)
University of Sofia, Bulgaria
July-August, 2013

10. **Laura Pitulice** (invited visitor)
West University of Timisoara, Romania
September, 2013

11. **Alexander Kaiser** (invited visitor)
Universität Innsbruck, Austria
September-December, 2013

12. **Prof. Jose A. Rodriguez** (invited visitor)
Brookhaven National Laboratory, USA
October, 2013

13. **Prof. Santiago Schnell** (invited visitor with the BKC excellence program)
University of Michigan Medical School, USA
November, 2013

14. **Prof. Jürgen Vogt** (invited visitor)
Universität Ulm, Germany
November, 2013

15. **Prof. Boutheina Kerkeni** (invited visitor)
Observatoire de Paris – Meudon, Paris, France
December, 2013

16. **Dr. Jaime Suárez Corujo** (invited visitor)
Universidad Autónoma de Madrid, Spain
December, 2013

III. SCIENTIFIC ACTIVITY OF IQTCUB MEMBERS

III.1 HIGHLIGHTS FROM MOST RELEVANT RESULTS

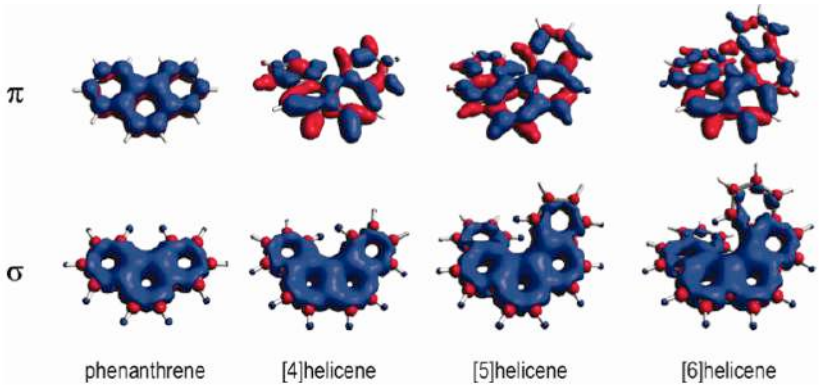
Here some of the most relevant results corresponding to every IQTCUB main research line are presented.

LINE 1. METHODS, ALGORITHMS AND COMPUTATIONAL TOOLS DEVELOPMENT

Pseudosymmetry Analysis of Molecular Orbitals.

D. Casanova, P. Alemany, A. Falceto, A. Carreras, S. Alvarez.

J. Comp. Chem., *34* (2013) 1321.



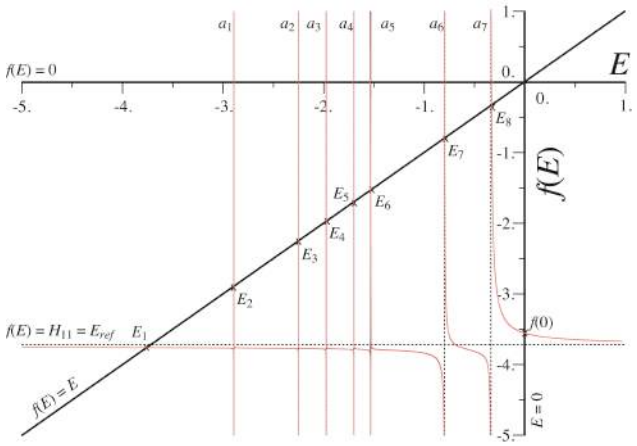
Lowest energy σ- and π-type bonding MOs for phenanthrene and [n]helicenes (n = 4–6)

We have developed a method to perform a pseudosymmetry analysis of molecular orbitals by means of the newly proposed irreducible representation measures. To do that we define first what we consider as molecular pseudosymmetry and the relationships of this concept with those of approximate symmetry and quasisymmetry. We develop a general algorithm to quantify the pseudosymmetry content of a given object within the framework of the finite group algebras. The obtained mathematical expressions are able to decompose molecular orbitals by means of the irreducible representations of any reference symmetry point group. The implementation and usefulness of the pseudosymmetry analysis of molecular orbitals is demonstrated in the study of σ and π orbitals in planar and non-planar polycyclic aromatic hydrocarbons and the t_{2g} and e_g character of the d-orbitals in the $[FeH_6]^{3-}$ anion in its high spin state along the Bailar twist pathway.

A Comparison Model Between Density Functional and Wave Function Theories by Means of the Löwdin Partitioning Technique.

M. Caballero, I. de P. R. Moreira, J. M. Bofill

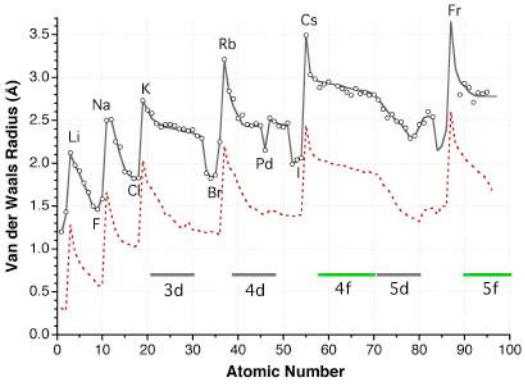
J. Chem. Phys., *138* (2013) 174107.



Qualitative representation of the Löwdin function *f(E)* for a *FCI* problem with *K* = *8* CSF's and $H_{1,1} = E_{ref}$, to show the general behaviour of this function.

A comparison model based in the Löwdin partitioning technique is used to analyze the differences between the wave function and density functional models. It is argued that density functional theory can be compared to the wave-function theory using the Löwdin function, f(E), at E = 0. The density functional theory can be seen as a special case of Löwdin function that does not satisfy all variational conditions on r(**r**) and also on the E_{XC}[r] term. This analysis shows that ignoring the restrictions imposed by the spin and space symmetry requirements the correlation expressed by the r(**r**) function will be inconsistent with a $g_1(\mathbf{r}_1;\mathbf{r}_1')$ function derivable from a spin and space symmetry adapted wave function $\Psi(\mathbf{r}_1 s_1,\cdots,\mathbf{r}_n s_n)$. The comparison scheme also provides a new insight on the variational requirements in order to achieve a consistent description of the molecular electronic structure of both ground and excited states. Some numerical results are reported.

A Cartography of the Van der Waals Territory
S. Alvarez
Dalton Trans. *42* (2013), 8617-8636.



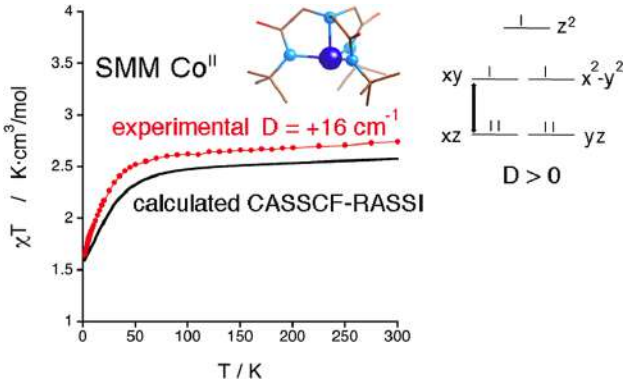
This article has presented a new set of van der Waals radii that shows consistent periodic trends (see Figure) and is expected to replace as a standard the commonly used Bondi radii.

LINE 2. COMPUTATIONAL MATERIALS SCIENCE

Mononuclear Single-Molecule Magnets: Tailoring the Magnetic Anisotropy of First Row Transition-Metal Complexes

S Gómez-Coca, E. Cremades, N. Aliaga-Alcaide, E. Ruiz

J. Am. Chem. Soc. *135* (2013), 7010-7018

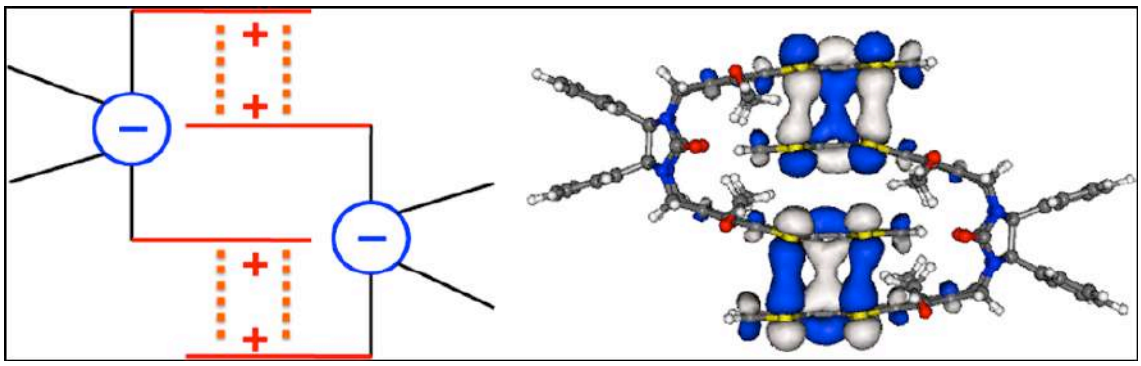


This is a combined computational and experimental study of the factors that determine the magnetic anisotropy of transition metal complexes, a crucial factor for taming their single molecule magnet behavior. In particular, it is shown that the magnetic anisotropy can be predicted based on the coordination number and electron configuration of the paramagnetic center. Based on such predictions, two cobalt complexes reported previously in the literature have been re-synthesized and magnetically characterized, and their predicted single molecule magnet nature has been confirmed.

Keys for the Existence of Stable Dimers of Bis-tetrathiafulvalene (bis-TTF)-Functionalized Molecular Clips Presenting $[TTF]^{\cdot+}\cdots[TTF]^{\cdot+}$ Long, Multicenter Bonds at Room Temperature

M. Fumanal, M. Capdevila-Cortada, J. S. Miller, J. J. Novoa.

J. Am. Chem. Soc. *135* (2013) 13814.

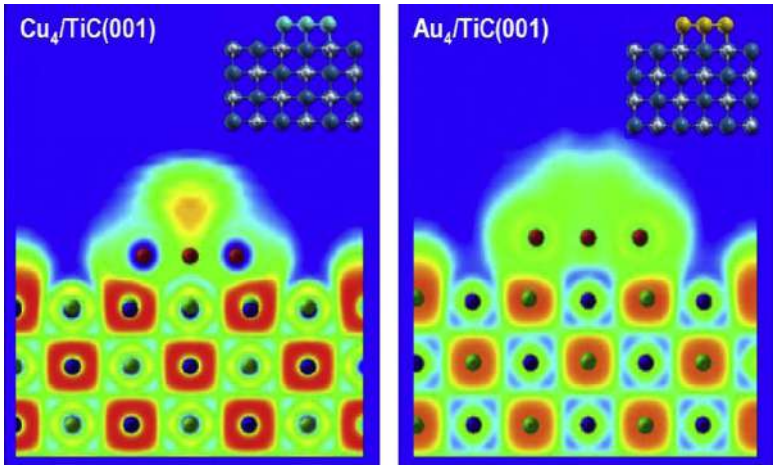


A computacional study has been performed to determine the keys governing the existence, in acetonitrile solutions, of dimers of (bis-TTF)-diphenylglycoluril molecular clips ($clip_2^{n+}$) that are stable at room temperature for n≤4. Electronic absorption studies suggested that they present $[TTF]^{l+}\cdots[TTF]^{m+}$ interactions at r.t.. We show that all $clip_2^{n+}$ n≤4 present an optimum geometry that has three short $[TTF]^{l+}\cdots[TTF]^{m+}$ interactions, and the computed ΔG(298K) matches the experimental data on the stability of these dimers. Our study traces the origin of their stability to (1) the zwitterionic character of their charge distribution, (2) the geometrical shape of the dimer, that allows the formation of two short contacts involving the + charged TTF group and the - charged central ring, (3) the presence of three short contacts among the TTF groups, which become two long bonds and one vdW interaction when the four TTF groups host a 1+ charge, and (4) the net stabilizing effect of the solvent.

CO_2 Hydrogenation on Au/TiC, Cu/TiC, and Ni/TiC Catalytst: Production of CO, Methanol, and Methane.

J.A. Rodriguez, J. Evans, L. Feria, A.B. Vidal, P. Liu, K. Nakamura, F. Illas

J. Catal., *307* (2013) 162.



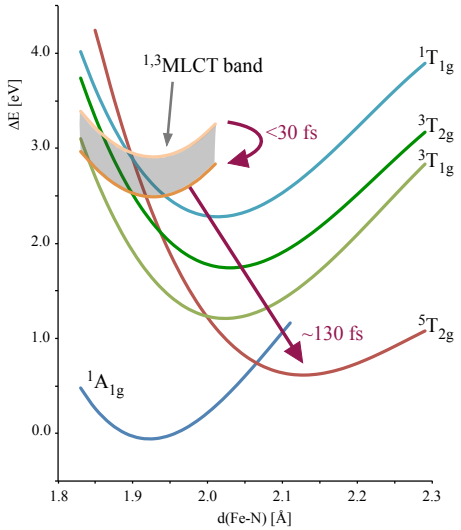
Electron-polarization plots for Cu_4 (left) and Au_4 (right) supported on TiC(001)

Small Au, Cu, and Ni particles in contact with TiC(001) display a very high activity for the catalytic hydrogenation of CO_2. The major product over these catalysts is CO which is produced by the reverse water–gas shift reaction (RWGS, $CO_2 + H_2 \rightarrow CO + H_2O$). In the cases of Au/TiC(001) and Cu/TiC(001), a substantial amount of methanol is also produced, but no methane is detected. Ni/TiC(001) produces a mixture of CO, methanol, and methane. The highest catalytic activity is found for small two-dimensional particles or clusters of the admetals in close contact with TiC(001). The catalytic activity of the supported metals can be orders of magnitude higher than those of Au(100), Cu(100), or Ni(100). Density functional calculations point to HOCO as a key intermediate for the generation of CO through the RWGS, with the production of methanol probably involving the hydrogenation of a HCOO intermediate or the CO generated by the RWGS.

Ultrafast Deactivation Mechanism of the Excited Singlet in the Light-Induced Spin Crossover of [Fe(2,2'-bipyridine)$_3$]$^{2+}$.

C. Sousa, C. de Graaf, A. Rudavskyi, R. Broer, J. Tatchen, M. Etinski, C. M. Marian

Chem. Eur. J. *19* (2013) 17541



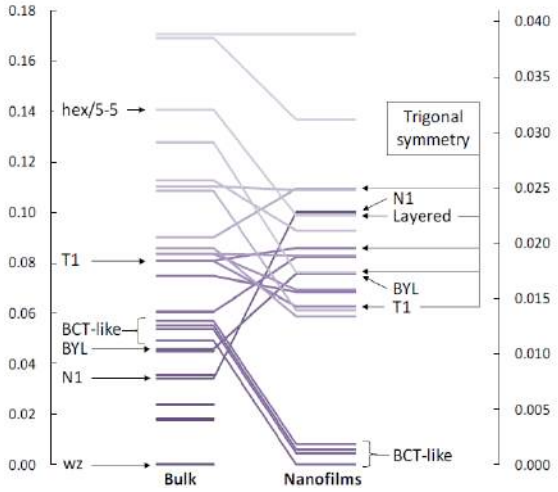
Deactivation process from the metal to ligand charge transfer band, MLCT.

The mechanism of the light-induced spin crossover of the [Fe(bpy)$_3$]$^{2+}$ complex (bpy = 2,2'-bipyridine) is studied by combining accurate electronic structure calculations and time-dependent approaches to calculate intersystem crossing rates. We determine all the intermediate electronic states along the pathway from low-spin to high-spin and give estimates for the deactivation times of the different stages. This strategy allows us to unravel the mechanism of the process. The calculations result in a total deactivation time on the same order of magnitude as the experimentally determined rate, in the range of 130 fs, and indicate that the complex can reach the final high-spin state via different deactivation channels. The optically populated excited singlet state rapidly decays to a triplet state with an Fe-d^6($t_{2g}^5 e_g^1$) configuration either directly or via a triplet MLCT state. This triplet ligand field state could in principle decay directly to the final quintet state, but a much faster channel is provided by internal conversion to a lower-lying triplet state and subsequent intersystem crossing to the high-spin state. The deactivation rate to the low-spin ground state is much smaller, in line with the large quantum yield reported for the process.

Nanofilm versus Bulk Polymorphism in Wurtzite Materials

I. Demiroglu and S. T. Bromley

Phys. Rev. Lett., 110 (2013) 245501.

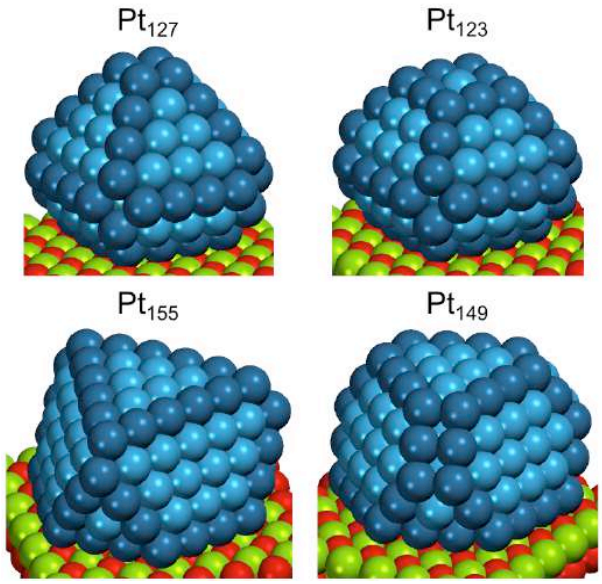


We find a rich low energy ZnO nanofilm polymorphism with a totally distinct stability ordering to that in the bulk. From this general basis we provide new insights into structural transitions observed during epitaxial growth and make predictions for nanofilm stability with varying strain or thickness.

Effect of MgO(100) support on structure and properties of Pd and Pt nanoparticles with 49-155 atoms.

S.M. Kozlov, H.A. Aleksandrov, J. Goniakowski, K.M. Neyman.

J. Chem. Phys., 139 (2013) 084701, 1-10



Platinum nanoparticles of different shape, size and orientation on MgO(100) support studied by means of density functional calculations.

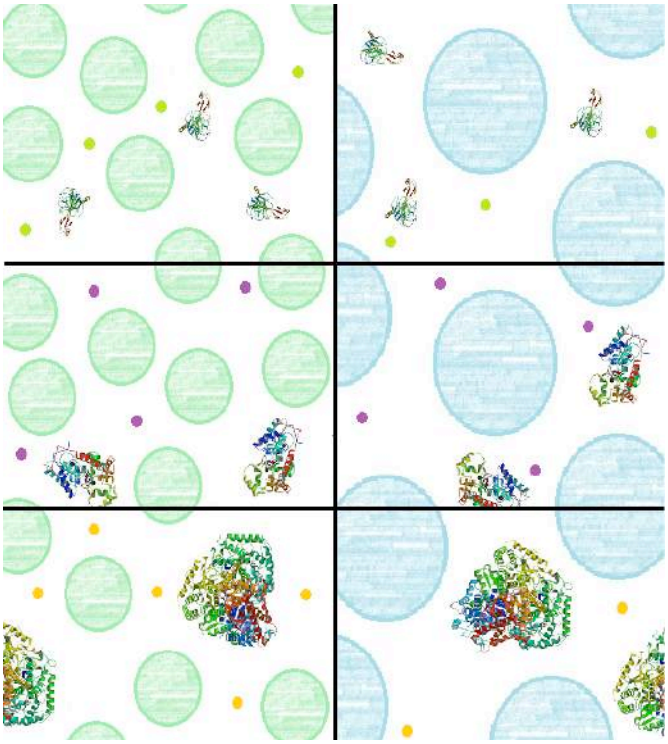
The computational study addressed the effect of an oxide support, MgO(100), on relative energies and various properties of Pd and Pt nanoparticles (NPs) that consist of up to 155 atoms (1.6 nm in size). While the support is found to significantly affect relative stabilities of NPs, other properties of NPs such as electronic structure and interatomic distances within NP do not notably change upon deposition. This is one of the first electronic structure studies, where the effect of oxide support on sizable metal nanoparticles was investigated. This work paves the way to more realistic modeling of such complex phenomena as metal-support interaction in heterogeneous catalysis.

LINE 3. COMPUTATIONAL BIOCHEMISTRY AND *SOFT MATTER*

Effect of crowding by Dextrans in enzymatic reactions

I. Pastor, C. Balcells, L. Pitulice, E. Vilaseca, S. Madurga, A. Isvoran, M. Cascante, F. Mas

Biophysical Chemistry, *185* (2013) 8



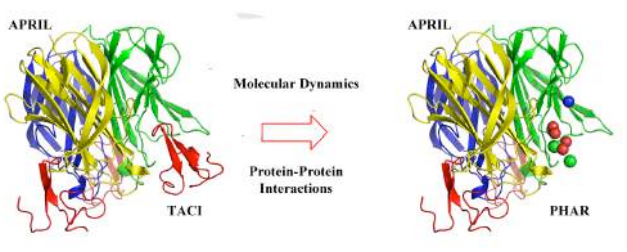
Effect of crowding on enzims of different size

The interior of the living cell is highly concentrated and structured with molecules that have different shapes and sizes. The consequences of such crowding upon enzymatic reactions remain unclear. In this paper we have studied and compared the kinetics of alpha-chymotrypsin, HRP and LDH. These reactions were chosen as model enzymatic processes occurring in different *in vitro* crowded media. The systems crowding has been built by introducing Dextran of several concentrations and sizes. Our results indicate that the volume occupied by the crowding agent, but not its size, plays an important role on the initial velocity of reactions involving tiny enzymes. However, the enzyme size is another important factor influencing the velocity of the reactions of large enzymes occurring in Dextran crowded media. In this situation, the reaction initial velocity depends on both occupied volume and dimension of the crowding agent that is present in the reaction media.

Structural analysis of the inhibition of APRIL by TACI and BCMA through molecular dynamics simulations

M. González-Mendióroz, A-B. Álvarez-Vázquez, J. Rubio-Martinez

J. Mol. Graph Model., *39* (2013) 13



Pharmacophore for the April-Taci interactions

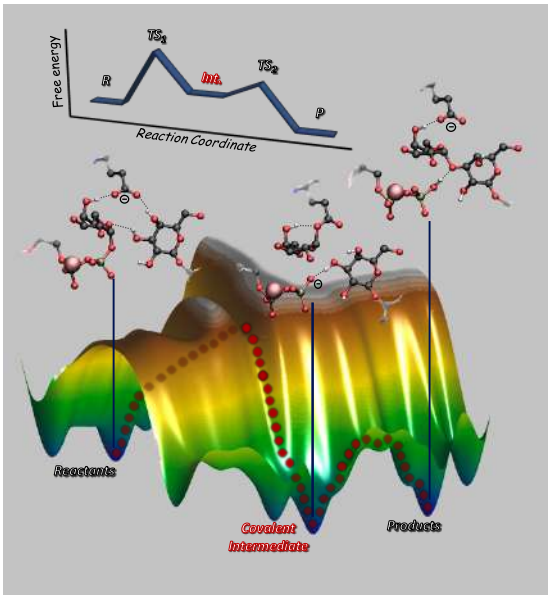
APRIL (A Proliferation-Inducing Ligand) is a member of the tumour necrosis factor (TNF) superfamily that binds the receptors (TNFRs) TACI and BCMA. There exists a great amount of evidence about the involvement of APRIL in autoimmune diseases and in different types of tumours where high mRNA levels have been detected. Thus, the design of compounds mimicking the inhibition of APRIL by its receptors seems to be a promising way to treat autoimmune and cancer diseases.

In this work, we report a detailed structural analysis of the inhibition of human and murine APRIL by its human receptors TACI and BCMA obtained by molecular dynamics simulations. New interactions are described that with those described experimentally can contribute to a better design of APRIL inhibitors. This is a first step towards the design of small compounds to inhibit the APRIL biological activity that is deregulated in many diseases

Formation of a covalent glycosyl-enzyme species in a retaining glycosyltransferase.

V. Rojas-Cervellera, A. Ardèvol, M. Boero, A. Planas, C. Rovira.

Chem. Eur. J. *42* (2013) 14018.



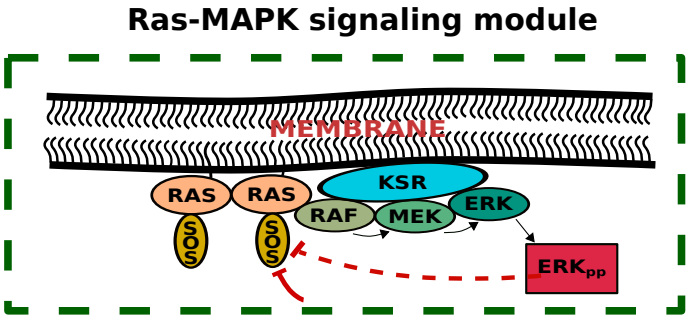
Molecular mechanism of glycosidic bond synthesis by the α3-galactosiltransferasa enzyme obtained by QM/MM methods.

Glycosyltransferases (GTs) are enzymes responsible for the formation of carbohydrates. Specifically, they synthesize glycosidic linkages by the transfer of a monosaccharide, from a sugar nucleotide donor to an acceptor substrate. GT alterations cause several diseases, such as infection, inflammation and several inherited disorders. One of the major challenges for the rational design of specific and potent drugs/inhibitors for this class of enzymes is unraveling their detailed reaction mechanisms, which still escape direct experimental probes. Using a combination of classical molecular dynamics simulations and QM/MM (quantum mechanics/molecular mechanics) metadynamics, we have trapped the long-time sought glycosyl–enzyme covalent intermediate of a retaining glycosyltransferase.

Negative feedback self-regulation contributes to robust and high-fidelity transmembrane signall transduction.

M.A. Serrano, M. Jurado, R. Reigada.

J. R. Soc. Interface, *10* (2013) 20130581.



Sketch of the Ras-MAPK signalling motif studied in the article. Two negative feedback controls in the motif are compared: external control (red sòlid line) and a self-regulation (red dashed line).

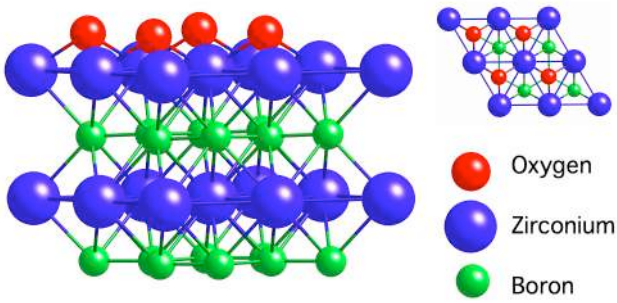
In this article we have presented a minimal motif model for transmembrane cell signalling based on the Ras-MAPK signalling pathway. The model assumes signalling events taking place in spatially distributed nanoclusters regulated by a birth/death dynamics. The combination of these spatio-temporal aspects can be modulated to provide a robust and highfidelity response behaviour without invoking sophisticated modelling of the signalling process as a sequence of cascade reactions and cycles, and fine-tuned kinetic parameters. Our results show that the fact that the distributed signalling events take place in nanoclusters with a finite lifetime regulated by local production is sufficient to obtain a robust and high-fidelity response. No external control of the signalling process is required to obtain a robust response.

LINE 4. REACTIVITY AND REACTIONS DYNAMICS

Elementary reaction processes involving atomic and molecular oxygen on ZrB_2 (0001) surface

P. Gamallo, R. Sayós

J. Phys. Chem. C *117* (2013) 5831.



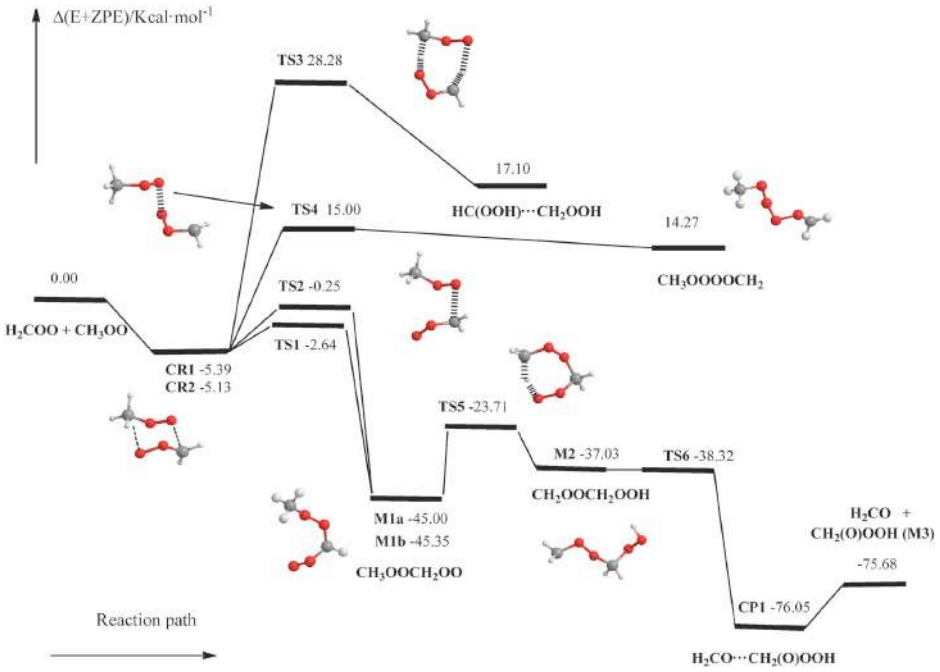
Atomic oxygen interacting with a ZrB_2 (0001) surface

The interaction of atomic and molecular oxygen along with the atomic recombination on thin ZrB_2(0001) Zr- and B-terminated surfaces were studied using density functional theory (GGA/PBE) calculations. The adsorption of atomic oxygen is predominantly produced on threefold hollow sites for the Zr-finished surface and on B–B bridge sites for the B-finished surface. The experimental specular HREELS loss peaks and their shifts at high O exposures can be satisfactory explained by the present calculations. The interaction of O_2 over both terminated surfaces produces mainly its dissociation through non-activated processes. This fact is in agreement with the observed open dissociation at room temperature. The atomic oxygen recombination over both ZrB_2 surfaces shows that the Eley-Rideal reaction will be much more important than the Langmuir-Hinshelwood reaction at all temperatures and even more accessible in the case of the B-finished surface.

The reaction of formaldehyde carbonyl oxide with the methyl peroxy radical and its relevance in the chemistry of the atmosphere

J.M. Anglada, S. Olivella, A. Solé

Phys. Chem. Chem. Phys., *15* (2013) 18921.



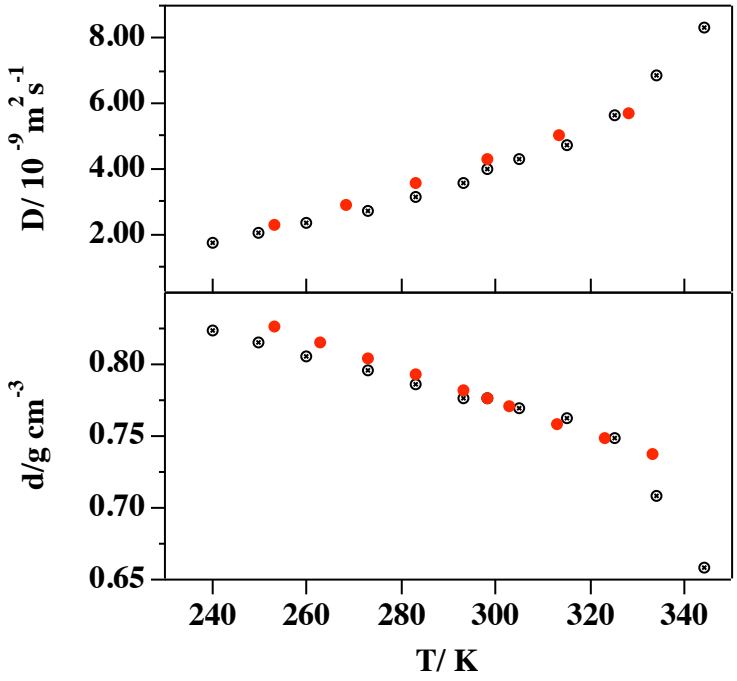
The reaction of formaldehyde carbonyl oxide (H2COO) with methyl peroxy radical (CH3OO), a prototype for the reactions of carbonyl oxides with alkyl peroxy radicals of potential interest in atmospheric chemistry, has been investigated by means of quantum-mechanical electronic structure methods (CASSCF, CASPT2, UQCISD, and UCCSD(T)) and DFT functionals (B3LYP, BH&HLYP, and M06-2X). Two reaction paths have been found for the lowest-barrier reaction, namely the CH3OO radical addition to the carbon atom of H2COO leading to the formation of the CH3OOCH2OO radical adduct. Both pathways begin with the formation of a pre-reactive complex with binding energies of 5.39 and 5.13 kcal·mol-1. The corresponding transition states are predicted to lie 2.64 and 0.25 kcal·mol-1 , respectively, below the energy of the reactants and the rate constant of the global reaction is calculated to be 3.74 x 10-12 cm3 molecules-1 s-1 at 298 K. Since the CH3OOCH2OO radical adduct is formed with an internal energy excess of about 45 kcal·mol-1, it can decompose unimolecularly into formaldehyde and the CH2(O)OOCH radical. This unimolecular decomposition involves an intramolecular H-atom transfer followed by the decomposition of the CH2OOCH2OOH radical intermediate. Kinetic calculations based on the collision-reaction master equation employing the MultiWell Program

Suite reveal that the CH3OOCH2OO radical adduct is stabilized in a 86.9%, whereas the 13.10% of the reaction corresponds to the formation of H2CO plus CH2(O)OOH radical. It is concluded that the methyl peroxy radical addition to substituted carbonyl oxides might be the source of low volatility oligomers observed in secondary organic aerosols in chamber studies.

A Model Potential for Acetonitrile: from Small Clusters to Liquid

M. Albertí, A. Amat, F. De Angelis, F. Pirani

J. Phys. Chem. B., *117* (2013) 7065.



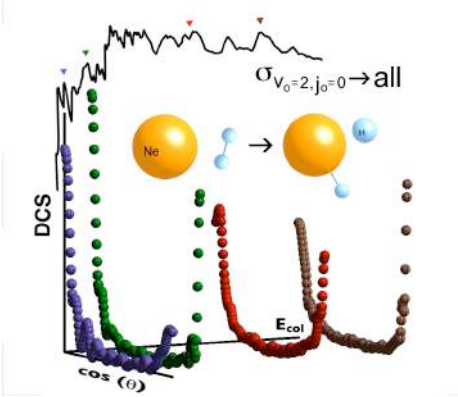
Mean diffusion coeficients (D) and density (d) for the pure acetonitrile obtained by means MD simulations using a NpT ensemble at several temperatures (N = 343, p = 1 bar) compared with experimental results (red circles)

The CH_3CN-CH_3CN and ion-CH_3CN (ion= Li^+, Na^+, K^+, I^-) interaction potentials, allowing the modelitation of both pure acetonitrile and its solutions, are presented. The interaction potentials have been constructed to be used in the study of dye-sensitized solar cells. The first step in the construction of the potential model is to assume the total separability of electrostatic and nonelectrostatic interactions, the late being represented by menas of the *Improved Lennard Jones* function, whose relevant parameters have been derived from values of the polarizability assigned to the ions and to different groups on the CH_3CN molecule, compatible with the whole molecular polarizability. By means of Molecular Dynamics simulations and the application of the interaction potential, small clusters of acetonitrile, $(CH_3CN)_{2,3,4}$, ion-acetonitrile clusters of the ion-$(CH_3CN)_{36}$ type and liquid acetonitrile have been investigated.

Resonances in the Ne + H_2^+ → NeH^+ + H Proton-Transfer Reaction.

P. Gamallo, F. Huarte-Larrañaga, M. González.

J. Phys. Chem. A, *117* (2013) 5393-5400



Combined plot of the excitation function and differential cross section as a function of the collision energy.

The Ne + H_2^+ → NeH^+ + H reaction is relevant in plasma physics and has been for a long time a benchmark system for triatomic reactions, attracting experimental and theoretical interest. One of the most appealing features is the presence of oscillations in the excitation function that could be eventually measured. In this publication, two groups of the IQTCUB joined efforts to investigate the oscillations found in the integral cross section of Ne + H_2^+, combining accurate time independent and time dependent quantum dynamics simulations. To do this we employed the best potential energy surface available, derived from *ab initio* MRCI calculations. From the analysis of our quantum dynamics simulations we proved that the oscillations correspond to true resonances which, arise from the influence of the global $[Ne\text{-}H\text{-}H]^+$ minimum on the dynamics. As most data available on resonances in bimolecular reactions correspond to neutral systems and heavy-light-heavy kinematics, the present results and the latest experimental progresses achieved in reaction dynamics will probably encourage the experimentalists to carry out higher resolution studies on this benchmark system.

III.2 PUBLICATION LIST

ARTICLES

1. *Structural analysis and insights into the glycon specificity of the rice GH1 Os7BGlu26 β-D-mannosidase.*
A. Tankrathok, J. Iglesias-Fernández, S. Luang, R. C. Robinson, A. Kimura, C. Rovira, M. Hrmova, J. Ketudat Cairns.
Acta Crystallogr. D *69* (2013) 2124

2. *Interconversion of Quadruply- and Quintuply-Bonded Dimolybdenum Complexes by Reductive Elimination and Oxidative Addition Reactions of Dihydrogen*
M. Carrasco, N. Curado, C. Maya, R. Peloso, A. Rodríguez, E. Ruiz, S. Alvarez, E. Carmona
Angew. Chem. Int. Ed. *52* (2013), 3227-3231.

3. *Evidence for Multicenter Bonding in Dianionic Tetracyanoethylene Dimers by Raman Spectroscopy.*
J. Casado, P. Mayorga Burrezo, F.J. Ramírez, J.T. López Navarrete, S.H. Lapidus, P.W. Stephens, H.-L. Vo, J.S. Miller, F. Mota, J.J. Novoa.
Angew. Chem. Int. Ed. *52* (2013) 6481-6485.

4. *Slow Magnetic Relaxation in a Co^{II}–Y^{III} Single-Ion Magnet with Positive Axial Zero-Field Splitting*
E. Colacio, J. Ruiz, E. Ruiz, E. Cremades, J. Krzystek, S. Carretta, J. Cano, T. Guidi, W. Wernsdorfer, E. K. Brechin
Angew. Chem. Int. Ed. *52* (2013), 9130-9134.

5. *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. (2013). In press (DOI: 10.1002/anie.201308334).

6. *Electroporation of heterogeneous lipid membranes.*
R. Reigada.
Biochimica et Biophysica Acta (2013), accepted.

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

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BOOK CHAPTERS AND PROCEEDINGS

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2. *Volume Editor's Introduction*
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III.3 OTHER ACTIVITIES

DOCTORALS THESES 2013

1. *De la superfície d'energia potencial a la reactivitat química*
Marc Caballero Puig
Facultat de Química, Universitat de Barcelona
November 2013

2. *Moléculas Funcionales y Nanotubos Funcionalizados*
Silvia Gómez Coca
Facultat de Química, Universitat de Barcelona
November 2013

3. *Estudio QM/MM del mecanismo y cinética de las reacciones de la proteasa NS3 del virus de la hepatitis C con sus sustratos principales*
José Ángel Martínez González
Departament de Química, Universitat de la Rioja
November 2013

4. *Transporte Cuántico y Magnetismo en Sistemas Inorgánicos: un Estudio Computacional*
Daniel Aravena Ponce
Facultat de Química, Universitat de Barcelona
December 2013

5. *Estudi teòric de la estereodinàmica de rotors i engranatges moleculars*
Abel Carreras Conill
Facultat de Química, Universitat de Barcelona
December 2013

6. *Estructura electrónica de sólidos inorgánicos*
Sergio Conejeros Espíndola
Facultat de Química, Universitat de Barcelona
December 2013

MASTERS THESES 2013

1. *Estructura Geométrica y Electrónica del Dianión de Benceno*
Andrés Falceto Palacín
Facultat de Química, Universitat de Barcelona
January 2013

2. *Estudi Teòric pel Disseny d'inhibidors de B-Raf. Preparació de nous agents potencialment inhibidors de B-Raf.*
Luis Eduardo Coronel Cordero
Màster Experimental en Ciències Farmacèutiques, Universitat de Barcelona
February 2013

3. *Structure based identification of inhibitors for TKTL1, a tumor specific transketolase-like protein.*
Hindujaraj Mannar Vijayanandaraj
Erasmus Mundus Masters – Bio-Health Computing, Universitat de Barcelona
June 2013

4. *Compuestos basados en Derivados Nitrogenados de la Heptacina*
Lindley Maxwell Villacorta
Facultat de Química, Universitat de Barcelona
July 2013

5. *Rational Design of new Monunuclear Single-molecule Magnets*
Jordi Trigueros Enguídanos
Facultat de Física, Universitat de Barcelona
July 2013

6. *Simulation of Intracellular protein diffusion using Brownian Dynamics*
Albert Ràfels
Facultat de Química, Universitat de Barcelona
July 2013

7. *La substitució nucleòfila interna: estudi computacional de la descomposició d'alquil clorosulfits per mitjà de càlculs estàtics i dinàmics.*
Lluís Raich
Facultat de Química, Universitat de Barcelona
September 2013

8. *H_2 confined in Single-walled Carbon Nanotubes: a MCTDH quantum dynamics study.*
Manel Mondelo Martell
Facultat de Química, Universitat de Barcelona
September 2013

9. *Estudi de l'estructura electrònica, l'enllaç i les propietats elèctriques de compostos de metalls de transició amb estructura tipus $NbAs_2$.*
Alberto Figueroba Sánchez
Facultat de Química, Universitat de Barcelona
September 2013

10. *Exploring efficient phosphorescence emission in purely organic materials.*
Clàudia Climent Biescas
Facultat de Química, Universitat de Barcelona
September 2013

11. *Docking, Molecular Dynamics Simulation and Free Energy Studies of the Binding Mechanism of Inhibitors with B-Raf, c-Abl and p38 Kinases.*
Ignacio Pasamontes Fúnez
Master in Bioinformatics for Health Sciences, Universitat Pompeu Fabra
2013

12. *Molecular Dynamics Simulation and Energy Calculation Studies of the Binding Mechanism of Inhibitors with c-Abl*.
Erim Yurci
Màster de Biotecnologia Molecular, Universitat de Barcelona
2013

SCIENTIFIC CONFERENCES AND MEETINGS 2013

Binational and National SCF Prizes (*Award Ceremony 2012*)
Société Chimique de France, Mulhouse (France)

Theoretical and Structural Exploration of the Van der Waals Territory
S. Alvarez (*conference*)

Journées de Modélisation
Paris (France)

Theoretical and Structural Exploration of the Van der Waals Territory
S. Alvarez (*conference*)

13th Conference of the Doctoral School
École Doctorale de Chimie Moléculaire de Paris Centre, Paris (France)

Molecular Symmetry and Pseudosymmetry: Some Concepts and Tools
S. Alvarez (*conference*)

Singlet Fission Workshop
Lyons (Colorado, USA)

RAS-SF: A simple and suitable approach for the electronic structure study of singlet fission
D. Casanova (*oral communication*)

8a Reunión Científica de Bioinorgánica
Burgos (Spain)

Oxidación de Complejos de Cobre(I) con Ligandos Benzimidazolilaminotioéter
P. R. Martínez-Alanis, G. Aullón, I. Castillo (*poster*)

SMASH- Small Molecule NMR Conference
Santiago de Compostela (Spain)

Representation and Abstraction: Art, Music and Chemistry
S. Alvarez (*invited conference*)

The Como Moments: Theoretical&Computational Modelling of Magnetically Ordered Molecules & Electronic Nano-Transport of Spins.
Como (Italy)

Ligand-Induced Changes of Magnetic Anisotropies in Transition Metal Complexes
Jordi Ribas (*oral communication*)

4th European Conference on Molecular Magnetism

Karlsruhe (Germany)

Dividing the spoils of the different magnetic behavior in the two phases of bistable (BDTA)2[Co(mnt)2] compound: the role of magnetic topology and g-tensor.
M. Deumal, S. Vela, J.J. Novoa, J. Ribas-Arino (*poster*)

Computational modeling of Molecular Magnetic Materials
S. Vela, J. Ribas-Arino, M. Deumal. J. J. Novoa (*poster*)

A theoretical Study of the Magnetic Properties of Benzotriazinyl-based Molecular Magnets
M .Fumanal, S. Vela, J. Ribas-Arino, J. J. Novoa (*poster*)

Workshop in honor of J. M. Tel
Salamanca (Spain)

Organizer of the workshop:
J.J. Novoa

Molecule-based Magnetism using Theoretical Methods
J.J. Novoa (*oral communication*)

Past, Present and Future of Crystallography @ Politecnico di Milano: From Small Molecules to Macromolecules and Supramolecular Structures
(Politecnico di Milano, Milano, Italy).

Intermolecular interactions in molecule-based magnets: Long distance bonds between radical-ions
J.J. Novoa (*invited conference*)

7th Workshop on Crystal Forms – Bologna
Università degli Studi di Bologna (Italy).

Bistable crystals: keys to their existence and polymorphic transformation
J.J. Novoa (*invited conference*)

3rd New trends in Computational Chemistry for Industry Applications
Barcelona (Spain)

Member of the organizing committee
F. Illas

Molecular dynamics study of CO over O-preadsorbed β–cristobalite surface
P. Gamallo, H. Prats, R. Sayós

Effect of crowding by Dextrans in enzymatic reactions
C. Balcells, I. Pastor, L. Pitulice, E. Vilaseca, S. Madurga, A. Isvoran, M. Cascante, F. Mas

Simulation of intracellular protein diffusion using Brownian Dynamics
A. Rafels, S. Madurga, I. Pastor, E. Vilaseca, M. Cascante, F. Mas

H adsorption and absorption in Pd nanoparticles supported on MgO(100).
S.M. Kozlov, H.A. Aleksandrov, K.M. Neyman

Dynamics of the $O(^3P) + HCD_3(v_1=0,1) \rightarrow OH + CD_3$ combustion reaction
R. Martínez, P. Gamallo, A. Vilà, M. González

Theoretical studies of enzymatic reactivity: The reaction of the HCV NS3/NS4A protease with the NS5A/5B substrate
J.A. Martínez, R. Martínez, M.P. Puyuelo, L. Masgrau, M. González

IVth IQTCUB Symposium
Barcelona (Spain)

Membre del comité organitzador
F. Illas

Spin crossover in Fe(II) systems
C. Sousa

Taming the activity of complex Pt/CeO_2 heterogeneous catalysts
A. Bruix

Atomic and electronic structure of F-doped TiO_2
J.O. Lamiel-Garcia, S. Tosoni, F. Illas

Polymorphism in ZnO: a comparison of 3D bulk and 2D nanoslabs
I. Demiroglu, F. Illas, S.T. Bromley

ZnO Surfaces: Description, H-Passivation and IR Spectroscopy
F. Viñes, O. Lamiel, F. Illas

Effect of crowding by Dextrans in enzymatic reactions
Balcells, I. Pastor, L. Pitulice, E. Vilaseca, S. Madurga, A. Isvoran, M. Cascante, F. Mas

Simulation of intracellular protein diffusion using Brownian Dynamics
A. Rafels, S. Madurga, I. Pastor, E. Vilaseca, M. Cascante, F. Mas

Hydrogen confined in Single.walled Carbon Nanotubes: a MCTDH quantum dynamics study
M. Mondelo Martell, F. Huarte-Larrañaga

Vuitena Trobada de Joves Investigadors dels Països Catalans
Andorra La Vella (Andorra)

Estudi dinàmic de reaccions moleculars de monòxid de carboni sobre sílice amb oxigen atòmic preadsorbit
H. Prats, P. Gamallo, R. Sayós

Efecte del crowding macroolecular en reaccions enzimàtiques
C. Balcells, I. Pastor, L. Pitulice, E. Vilaseca, S. Madurga, A. Isvoran, M. Cascante, F.

Mas

Disseny i síntesi de nous inhibidors enzimàtics amb potencial activitat antitumoral
A. Vinuesa, L. Navarro, V. Prieur. J. Rubio, R. Pouplana, G. Guillaumet, MD. Pujol.

Quantum Reactive Scattering (QRS13)
Bordeaux (France)

Resonances in the proton transfer reaction Ne + H_2^+ → NeH^+ + H. A challenge for the experiment.
M. González, P. Gamallo, F. Huarte-Larrañaga

Non adiabatic quantum dynamics of the N + H_2 and O + H_2^+ isoelectronic systems
P. Gamallo, R. Martínez, P. Defazio, C. Petrongolo, M. Paniagua, M. González

Understanding the effect of vibrational excitation in Ne + H_2^+ (v=0-17,j=1) → NeH^+ + H, Ne + H^+ + H.
P. Gamallo, R. Martínez, J.D. Sierra, M. González

QCT dynamics of the OH + D_2 ⟶ HOD + D benchmark reaction in a quantum spirit
J.D. Sierra, L. Bonnet, M. González

XII Iberian Meeting on Atomic and Molecular Physics (IBER2013)
Universidad Pablo de Olavide, Sevilla (Spain)

Quasi-classical trajectory dynamics study of the OH + D_2 and O + HCD_3 benchmark combustion reactions
J.D. Sierra, L. Bonnet, R. Martínez, P. Gamallo, A. Vilà, M. González

Resonances and non-adiabatic processes in the Ne + H_2^+ and O + H_2^+ reactions.
M. González, P. Gamallo, F. Huarte-Larrañaga, M. Paniagua, P. Defazio, C. Petrongolo

Rate constants of the HCV NS3/NS4A protease reactions
J. A. Martínez, R. Martínez, L. Masgrau, M. González

Ultracold ^{4}He nanodroplets doped with O and O_2
A. Vilà, M. González, R. Mayol

Molecular states of the Li^+ + H + H system: nuclei dynamics in the BO approximation
J.M. Randazzo, A. Aguilar, F. Huarte, M. Albertí and J.M.Lucas

Reactive dynamics of the Li^+ + H_2 ⟶ LiH^+ + H collisions
J.M. Randazzo, A. Aguilar, F. Huarte, M. Albertí and J.M.Lucas

5th Iberian Meeting on Colloids and Interfaces, RICI5
San Sebastian (Spain)

Dissolution of ZnO nanoparticles in aqueous media: A first essential step in nanotoxicological studies
C. Rey-Castro, C. David, S. Cruz-González, J. Salvador, F. Mas, J. Puy, J. Galceran

Effect of mixed crowding media on the diffusion of alpha-chymotrypsin
I. Pastor, E. Vilaseca, S. Madurga, J.L. Garcés, M. Cascante, F. Mas

XVIIIth Meeting of the Reference Network of Theoretical and Computational Chemistry in Catalonia
CRAG, Campus UAB, Barcelona (Spain)

Simulació de la difusió de proteïnes intracel·lulars usant dinàmica browniana
A. Rafels, S. Madurga, I. Pastor, E. Vilaseca, M. Cascante, F. Mas

Effect of MgO support on structures and H ad-/absortion properties of Pd and Pt nanoparticles
S. M. Kozlov

Ion-Molecule Reactions with alkali metals
E.López, J.Aguilar, J.M.Lucas, J. de Andrés, M. Albertí and A. Aguilar

27th ECIS
Sofia (Bulgaria)

Molecular dynamics simulation of the spherical electrical double layer of a soft nanoparticle
S. Madurga, M. Nedyalkova, S. Pisov, I. Pastor, E. Vilaseca, F. Mas

The role of citrate in the stabilization of gold nanoparticles. Conformational analysis of citric acid
M. Nedyalkova, S. Madurga, S. Pisov, I. Pastor, E. Vilaseca, F. Mas

Ceria Symposium 2013
Barcelona (Spain)

Member of the organizing committee
F. Illas

Strong Metal-Support interactions in Pt/CeO_2 heterogeneous catalysts.
A. Bruix

Steps on CeO_2(111): Characterization and O vacancy formation.
S.M. Kozlov

2nd Annual Spain Supercomputing Conference
Barcelona (Spain)

Testing Au/TiC as a potential catalyst for CO_2 hydrogenation
F. Illas

Theoretical Chemistry in Spain told by women.
Tarragona (Spain)

Spin states in Fe(II) systems
C. Sousa

7th Molecular Quantum Mechanics 2013. Electron Correlation: The Many-body problem at the Heart of Chemistry.
Lugano (Switzerland)

A Comparison Model Between Density Functional and Wave Function Theories by Means of the Löwdin Partitioning Technique
J. M. Bofill, I. de P.R. Moreira, M. Caballero.

Large Matrix Diagonalization Algorithms Based on Lagrange-Newton-Raphson Schemes: Effective Krylov Space LNRd routine
I. de P.R. Moreira, J. M. Bofill

Royal Golden Jubilee PhD (RGJ-Ph.D).Congress XIV
Pattaya (Thailand)

Modeling complex systems from first principles: The water gas shift reaction on Pt/ceria catalyts
Francesc Illas

XXXIX International Conference of Theoretical Chemist of Latin Expression
Granada(Spain)

Prediction of Optical Excitation Energies of Bulk Oxides from Density Functional Theory and Quasi Particle Calculations
Sergio Tosoni and Francesc Illas

Theoretical study of CO oxidation by Cu, Ag and Au nanoparticles and extended surfaces
S. G. Otero, B. Pascucci, F. Illas, M. M. Branda, P. G. Belelli

Density Functional Theory bases study of metanol adsorption and decomposition on low index Miller CeO_2 surfaces
M.M. Branda, A. Bruix, F. Illas

Density Functional Theory based study of NO2 reduction by Cu, Ag and Au: nanoparticles versus extended surfaces
B. Pascucci, G. S. Otero, P. G. Belelli, F. Illas, M.M. Branda.

Annual Meeting of COST 1104 action: Reducible oxide chemistry, structure and functions
Uppsala (Sweden)

Management committee
Francesc Illas

Oxygen vacancy formation on steps on CeO_2(111).
S.M. Kozlov, K.M. Neyman

Electronic structure and absolute energies of steps on CeO_2(111).

S.M. Kozlov, F. Viñes, N. Nilius, S. Shaikhutdinov, K.M. Neyman

Substrate mediated diversity in Pt-CeO_2 interactions.
A. Bruix, F. Illas, K.M. Neyman

Ionic Pt-CeO_2 composites for fuel cells applications: Combined experimental and density-functional studies.
K.M. Neyman

WG1/WG3 Meeting of the COST Action CM1104 "Reducible oxide chemistry, structure and functions"
TU Vienna, Vienna (Austria)

Distinguishing different Pt sites in Pt/CeO_2 via CO adsorption: A DFT study.
H.A. Aleksandrov, P.S. Petkov, K.M. Neyman, G.N. Vayssilov

Steps on CeO_2(111): Step energies, STM appearance, O vacancy formation.
K.M. Neyman

On the concept of ionic platinum species in catalytic materials based on Pt-CeO_2
K.M. Neyman

Convergent Distributed Environment for Computational Spectroscopy
CoDECS 2013 Workshop
San Lorenzo de El Escorial (Spain)

Electronic structure and properties of F-doped titania
S. Tosoni, O. Lamiel-Garcia, F. Illas

Atomic and electronic structure of F-doped TiO2 bulk and surfaces
O. Lamiel-Garcia. S. Tosoni, F. Illas

On the low lying magnetic states of organic diradicals with phenyl bridges
D. Reta, I. de P.R. Moreira, F. Illas, A. K. Pal, S. N. Datta

Frontiers in Modelling Optical Excitations of Materials
Chicheley (United Kingdom)

Optical Excitations in Bulk Oxides from Density Functional Theory and Quasi Particle Calculations
S. Tosoni and F. Illas

18 Quantum System in Chemistry and Physics
Paraty (Brazil)

Towards ab initio modeling of doped high Tc superconducting cuprate parent compounds
Francesc Illas

Laboratory Astrophysics 2013

Kassel (Germany)

Initial Stages of Silicate Dust Nucleation: Bottom-up Insights from Computational Modelling
S. T. Bromley

LASSIE 2013 Summer School: State-of-the-art Astrochemistry
París (France)

1.) Structure of Nanoscale Dust Precursors, 2.) A Bottom-up Approach to Dust Nucleation: Nano-silicates, 3.) Calculating Surface Energies and Absorption Energies: VASP
S. T. Bromley

Theory of Atomic and Molecular Clusters VII
Birmingham (United Kingdom)

Nucleation of Nanosilicate Clusters: from the Interstellar Medium to Aqueous Solution
S. T. Bromley
Density-functional modelling of CeO2 nanoparticles: Structure, oxygen mobility and interactions with adsorbed molecules and metal species.
K.M. Neyman

Deutsche Physikalische Gesellschaft Spring Meeting of the Condensed Matter Section 2013
Regensburg (Germany)

Bandgap Engineering via Nanoporosity in ZnO
I. Demiroglu, S. Tosoni, F. Illas, S. T. Bromley

19th International Vacuum Congress IVC-19
Paris (France)

Competing Mechanisms of Catalytic H2 Formation and Dissociation on an Ultrasmall Silicate Nanocluster Dust Precursor
B. Kerkeni, S. T. Bromley

International Symposium on Atomic Cluster Catalysis
Tsinghua University, Beijing (China)

Density-functional modelling of CeO_2 nanoparticles.
K.M. Neyman

China-Europe International Workshop on Alloy Nanoparticles
Beijing (China)

Density-functional modelling of mono- and bimetallic nanoparticles relevant to catalysis.
K.M. Neyman, S.M. Kozlov

I Jornada d'Investigadors Predoctorals Interdisciplinària (JIPI)

Universitat de Barcelona, Barcelona (Spain)

Computational Chemistry for Nanostructuring Effects in Heterogeneous Catalysis.
S. M. Kozlov

An Experimental and Theoretical point of view of Ion-Molecule Reactions
E. López, J. Aguilar, J.M. Lucas, J. de Andrés, M. Albertí, A. Aguilar

International Summer School on Basic Concepts and First-Principles Computations for Surface Science: Applications in Chemical Energy Conversion
Nordeney (Germany)

H adsorption and absorption in Pd nanoparticles supported on MgO and unsupported Pd nanoparticles: Is consideration of a substrate always a must?
S.M. Kozlov, K.M. Neyman

International Conference on Computer Science ICCS 2013 / 7th Workshop on Computational Chemistry
Barcelona (Spain)

Performance analysis of two quantum reaction dynamics codes: Time-dependent and time-independent strategies
P. Gamallo, M. González, F. Huarte-Larrañaga

Quantum Scattering of the Ne + H2+ reaction: Comparison of TD and TI computational tools
F. Huarte-Larrañaga, M. González, P. Gamallo

9th EBSA European Biophysics Congress
Lisboa (Portugal)

QM/MM study of HCV NS3/NS4A protease with its main substrates: from the structure to the kinetics
J. A. Martínez, R. Martínez, M.P. Puyuelo, L. Masgrau, M. González

V Jornadas de Jóvenes Investigadores en Física Atómica I Molecular
Madrid (Spain)

Reacciones Ion-Molécula con Metales Alcalinos
E. López, J. Aguilar, J.M. Lucas, J. de Andrés, M. Albertí, A. Aguilar

XXV International Symposium on Molecular Beams (ISMB 2013)
Prague (Czech Republic)

Gas Phase Dehydrohalogenation Reactions of Halogenated Organic Compounds Induced by Collisions with Alkali Ions (Li^+, Na^+ and K^+)
J. Aguilar, J.M. Lucas, J. de Andrés, F. Huarte, M. Albertí, D. Bassi and A. Aguilar

Hybrid Quantum Mechanics / Molecular Mechanics (QM/MM) Approaches to Biochemistry (and beyond)

CECAM-EPFL Lausanne (Switzerland)

Member of the organizing committee of the school
Carme Rovira

EMBO conference - Spatial 2013: From Spatial Signaling to Sensing Spatiality
Dead Sea (Israel)

Negative-feedback self-regulation contributes to high-fidelity transmembrane signal transduction (poster and oral communication)
M. Jurado, R. Reigada

IX Seminarios de Estudios Avanzados en Diseño Molecular y Bioinformática
Varadero (Cuba)

Analyzing the Electronic Structure of Molecules Using Continuous Symmetry Measures (invited conference)
P. Alemany

Electronic Properties of Covellite (CuS) (poster)
S. Conejeros, I. Ribeiro, M. Llunell, P. Alemany

Computational Study of D-π-A Organic Dyes for Dye Sensitized Solar Cells (poster)
C. Climent, D. Casanova

RESEARCH STAYS ABROAD

F. Illas **Indian Institute of Technology, Mumbai (India)**

Visit within the framework of a India-Spain bilateral program. January 2013

K.M. Neyman **Nanyang Technological University, Singapore**

Invited associate visiting Professor, School of Chemical and Biomedical Engineering. February-March 2013

S.M. Kozlov **University of Genova, Genova (Italy)**

Predoctoral research stay. March-April 2013

M. Albertí **Università di Perugia, Perugia (Italy)**

Visiting Professor, Dipartimento di Chimica. April-July 2013.

S. Madurga **Sofia University, Sofia (Bulgaria)**

Invited Visiting Professor, Chemistry Faculty. May 2013

C. Sousa **University of Groningen, Groningen (The Netherlands)**

Invited Visiting Professora, Department of Chemical Physics and Zernike Institute for Advanced Materials. July 2013.

K.M. Neyman **University in Prague, Prague (Czech Republic)**

Invited visiting scientist. July-August 2013

K.M. Neyman **Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen (Germany)**

Invited visiting scientist, School of Chemical and Biomedical Engineering. July-August 2013

J. J. Novoa **Clark University, Worcester (MA, USA)**

Invited Visiting Professor, School of Chemistry. September-October 2013

M. Mondelo **Universität Bielefeld (Germany)**

Predoctoral research stay. October 2013

M. Albertí **Università di Perugia, Perugia (Italy)**

Visiting Professor on sabbatical, Dipartimento di Chimica. September-December 2013.

E. López **Università di Trento, Trento (Italy)**

Predoctoral research stay, Dipartimento di Fisica. October-December 2013.

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

Grup d'Estructura de Materials Moleculars (GEM2)
Juan J. Novoa, Universitat de Barcelona
2009SGR-1203, 2009-2013
Agència de Gestió d'Ajuts Universitaris i de Recerca, Generalitat de Catalunya

Fisicoquímica de sistemes macromoleculars d'interès ambiental
Jaume Puy Llorens, Universitat de Lleida
2009SGR-465, 2009-2013
Agència de Gestió d'Ajuts Universitaris i de Recerca, Generalitat de Catalunya

Laboratorio de Ciencia de Materiales Computacional
Francesc Illas Riera, Universitat de Barcelona
2009SGR-1041, 2009-2013
Agència de Gestió d'Ajuts Universitaris i de Recerca, Generalitat de Catalunya

Química Teòrica i Computacional
Santiago Olivella Nel.lo, CSIC
2009SGR-1472, 2009-2013
Agència de Gestió d'Ajuts Universitaris i de Recerca, Generalitat de Catalunya

Dinàmica de reaccions químiques
Antonio Aguilar Navarro, Universitat de Barcelona
2009SGR-17, 2009-2013
Agència de Gestió d'Ajuts Universitaris i de Recerca, Generalitat de Catalunya

Grup de recerca consolidat d'estructura de proteïnes
Miquel Coll Capella, Consell Superior d'Investigacions Científiques (CSIC)
2009SGR-1309, 2010-2013
Agència de Gestió d'Ajuts Universitaris i de Recerca, Generalitat de Catalunya

Grup de Bioquímica Integrativa.
Jaime Rubio Martínez . Marta Cascante Serratosa. Universidad de Barcelona.
2009SGR1308, 2009-2013
Agència de Gestió d'Ajuts Universitaris i de Recerca. Generalitat de Catalunya.

Xarxa de Referència d'R+D+I en Química Teòrica i Computacional (XRQTC)
Francesc Illas Riera, Universitat de Barcelona
2013
Departament d'Innovació, Universitats i Empresa. Generalitat de Catalunya

Estructura electrónica y propiedades de moléculas y sólidos inorgánicos.
Eliseo Ruiz Sabin i 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)

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)

Dinámica de procesos químicos mediante haces moleculares y métodos teóricos.
Antonio Aguilar Navarro, Universitat de Barcelona
CTQ2010-16709
Ministerio de Ciencia en Innovación

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

Fisicoquímica de las interacciones de ligandos con polilectrolitos de interés ambiental y fisiológico
Francesc Mas Pujadas, Universitat de Barcelona
CTM2012-39183, 2013-2017
Dirección General de Investigación y Gestión del Plan nacional de I+D+I (MICINN)

Modelización ab initio de materiales de importancia tecnológica basados en óxidos, metales y las combinaciones de ambos: de la escala nanométrica al sistema extendido
Francesc Illas Riera, Universitat de Barcelona
FIS2008-02238, 2009-2013
Dirección General de Investigación y Gestión del Plan nacional de I+D+I (MICINN)

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)

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)

Dinámica cuántica de reacciones en sistemas poliatómicos y modelización de fisisorción de gases en nanoestructuras
Fermín Huarte Larrañaga, Universitat de Barcelona
CTQ2009-12215, 2009-2013 (prorrogat)
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.

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)

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

Asessorament en projectes de fotocatàlisis
Francesc Illas Riera
INAEL, 2011-2013

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
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