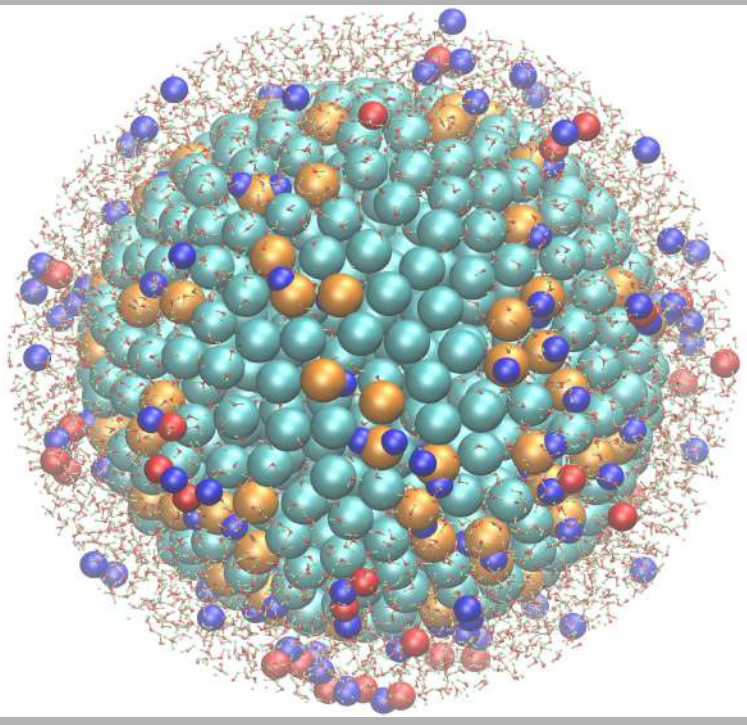
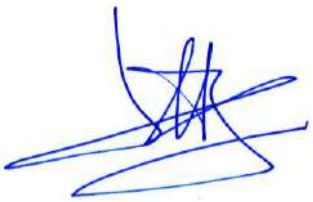
Institute of Theoretical and Computational Chemistry of Universitat de Barcelona (IQTCUB)



Memoir 2012

One can really state that 2012 has been the year where the Institute of Theoretical Chemistry of the *Universitat de Barcelona* (IQTCUB) has reached maturity in both organization and scientific aspects. As a reflection of this, the organization of research lines has been rationalised to better integrate the constituent research teams. Officially, IQTCUB was created on November 27th, 2007 by decision of the Board of Government of the *Universitat de Barcelona* (UB). Our institute 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 modelling). 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" which typically "resides" inside supercomputers with 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.

In the past few years and in spite of the world wide economic crisis, institutional support from UB has not been lacking. The continuous support from the Research Vicerector has been invaluable and we would like to fully acknowledge it. This support has allowed us to maintain and even improve a computational infrastructure where IQTCUB professors and researchers carry out high quality competitive scientific research. The following Research Memoir, including the new research line reorganization mentioned above, 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. In the years to come we look forward to further showing the worthiness of our Institute which is clearly fully deserving the support of an ambitious high quality university such as ours.



Francesc Illas
Director de l'IQTCUB

MEMOIR 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 68 Professors and Researchers, the full list is provided below with indication of the academic situation and affiliation within UB..

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	PCB / Organic Chemistry

Postdoctoral contracts

Juan de la Cierva contract

Pastor del Campo	Isabel	Physical Chemistry
Viñes Solana	Francesc	Physical Chemistry

Ramón y Cajal contract

Casanova Casas	David	Physical Chemistry
Ribas Ariño	Jordi	Physical Chemistry
Serrano Moral	Mariangels	Physical Chemistry

Other

Aleksandrov	Hristiyan A.	Physical Chemistry
D'Oria	Emiliana	Physical Chemistry
Dos Santos Politi	Jose Roberto	Physical Chemistry
Morón Tejero	Victor	Physical Chemistry
Suarez Corujo	Jaime	Physical Chemistry
Tosoni	Sergio	Physical Chemistry

Ph D students

FPI (Associated to Ministerio Research Grants)

Aguilar Fargas	Javier	Physical Chemistry
Bruix Fusté	Albert	Physical Chemistry
Caballero Puig	Marc	Physical Chemistry
Carreras Conill	Abel	Physical Chemistry
Jurado Sáez	Manuel	Physical Chemistry
Vela Llausi	Sergi	Physical Chemistry

FPU (Spanish Ministerio Program)

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

UB own program

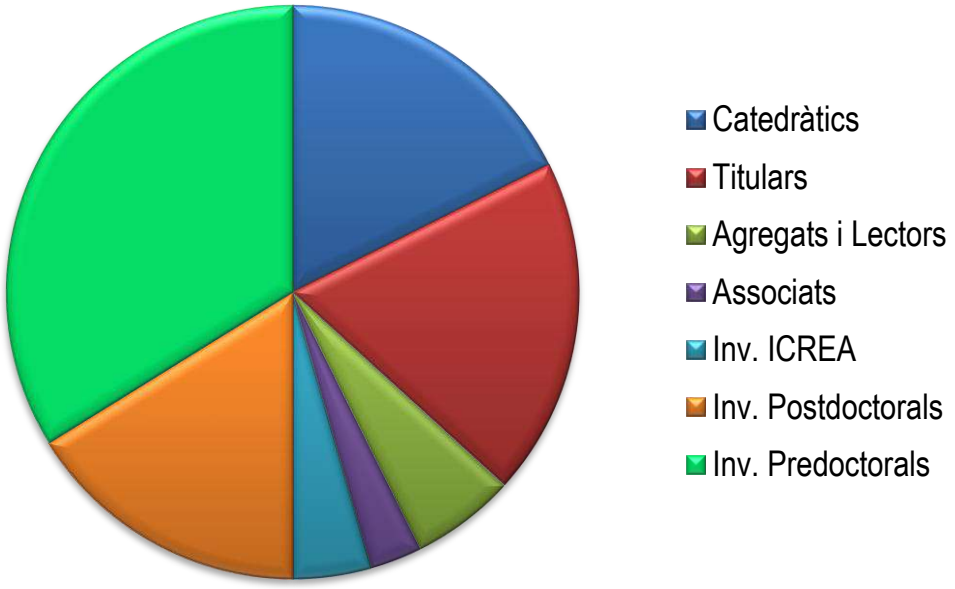
Fumanal Quintana	Maria	Physical Chemistry

FI (Catalan Government Program)

López Marne	Estefanía	Physical Chemistry
Vilà Casanovas	Arnau	Physical Chemistry

Other funding

Aravena Ponce	Daniel	Inorganic Chemistry
Climent Biescas	Clàudia	Physical Chemistry
Conejeros Espíndola	Sergio	Physical Chemistry
Demiroglu	Ilker	Physical Chemistry
Falceto Palacín	Andrés	Inorganic Chemistry
Iglesias Fernández	Javier	PCB
Lamiel Garcia	J. Oriol	Physical Chemistry
Maxwell	Lindley	Inorganic Chemistry
Moix Teixidor	Marc	Physical Chemistry
Reta Mañeru	Daniel	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 five calculation clusters located in a conditioned room of the Chemistry Faculty of UB. This room is cooled by two air conditioning machines of 47,000 and 66.000 KW respectively.

CALCULATION CLUSTERS

cerqt2 (approximate value 400.000 €)

Machine type	SUN cluster (4 racks)
Operating system	Red Hat Enterprise Server 2.1 (23 bits nodes) and Suse 9.2 (64 bits nodes)
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) + 2 100 lom cards (internal administration network, IAM)

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) + 2 100 lom cards (IAM)

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 de 2 with 1x73GB and 1x300GB hard disk respectively
Network: 2 gigabit network cards (calculation network) + 2 100 lom cards (IAM)

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) + 2 100 lom cards (IAM)

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 (IAM)

iqtc02 (approximate value 78.000 €)

Machine type HP cluster
Operating System Suse Linux Enterprise Server 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 (IAM)

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 (IAM)

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 (IAM)

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 (IAM)

iqtc03 (approximate value 33.000 €)

Machine type	HP cluster
Operating System	Suse Linux Enterprise Server 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 (IAM)

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 (IAM)

iqtc04 (approximate value 460.000 €)

Machine type	HP cluster
Operating system	Suse Linux Enterprise Server SLES11
Services	Calculation cluster
Structure	101 nodes
Notes	64 bits processors. Infiniband network
Specifications	

93 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)

2 INTEL HP ProLiant DL160 G6 nodes
CPU: 2x2.66GHz Xeon SixCore
RAM: 24GB
HD: 2x1TB 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 (IAM)

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 (IAM)

iqtc05 (approximate value 32.000 €)

Machine type	SGI Cluster
Operating System	Suse Linux Enterprise Server 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 (IAM)

SERVERS

GPU Server (approximate value 1.500 €)

Machine type	1 desktop node

Operating System Suse Linux Enterprise Server SLES11
Services GPU calculation
Structure 1 node
Specifications

Node
CPU: 1x3.06GHz Intel Core i7 950
RAM: 16GB
HD: 1x1TB hard disk
Network: 1 gigabit network (internal network)

Glusterfs disk server (approximate value 35.000 €)

Machine type Heterogeneous cluster (DELL+HP)
Operating system Suse Linux Enterprise Server SLES 10.2 (DELL cluster) + Suse Linux Enterprise Server SLES 11 (HP)

Services Storage service cluster with 32TB of space for user's data exported by GlusterFS
Structure 6 nodes
Notes Storage service with a dedicated UPS and redundant power supply
Specifications

5 DELL PowerEdge 2950 nodes
CPU: 2x2.50GHz Xeon QuadCore E5540
RAM: 8GB
HD: 1x80GB hard disk + 4x1TB (raid 5)
Network: 2 gigabit network card (internal network)

1 HP ProLiant DL180 G6 node
CPU: 2x2.27GHz Xeon QuadCore E5520
RAM: 56GB
HD: 12x2TB (raid 5)
Network: 2 gigabit network card (internal network)

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 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 2.300 €)

Machine type	2 redundant HP ProLiant DL120 G5 nodes
Operating system	Debian stable
Services	Xen, DRBD, IQTCUB internal services
Structure	2 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 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	Suse Linux Enterprise Server SLES10
Services	Server for the use of graphical applications (gaussview, p4vasp, etc.)
Structure	1 node
Notes	Server connected with a UPS
Specifications	
	1 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 in 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)
- 3 Switchs Layer 2 HP with 48 ports (internal network for iqtc04 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)

The approximated total cost of this equipment is 30.000€

SUMMARY

Processors..... 2306 CPUs

Memory.....7624 GB RAM

Calculation disk capacity ..... 144.332 TB

Data user disk capacity..... 32 TB

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

1.532.600 €*

Mr. Jordi Inglés, IQTCUB's System responsible with one of the institute calculation cluster.

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

II. IQTCUB ACTIVITIES

II.1 GENERAL ACTIVITIES

Next, a description of activities and actions promoted by IQTCUB through 2012 is provided..

a. *3rd IQTCUB workshop*. This one day workshop aimed at presenting the IQTCUB progress in research lines took place on November 23rd , 2012. The IQTCUB members and some internationally well recognized speakers present the most recent work. This year we highlight the participation of Prof. Ignasi Nebot from the *Universitat de Valencia* as well as that of Prof. Ricard Gelabert from *Universitat Autònoma de Barcelona* and Prof. Lluïs Blancafort from *Universitat de Girona*. The IQTCUB budget was use to cover the traveling expenses Prof. Nebot and Prof. Dr. Blancafort as well as the cattering service offered to all assistants.

   Total cost: 900 €

b. Promotion and encouragement of research. This year the IQTCUB has offered a total of three 1800 € 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; the main aim being 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. Clàudia Climent Biescas and Mr. Manel Mondelo Martell and Mr. Luís Adrián Raich Armendáriz.

   Total cost: 5.400 €

c. *Introductory course in Computational Chemistry*. The main goal of this course is to broaden the knowledge of chemistry undergraduate students in applied informatics and Computational Chemistry. The curs takes place along a whole week and is mainly addressed to Chemistry and Chemical Engineering students at UB. The 2012 edition is the second one and has been very successful with almost 40 student registered. The corse took place during june 25-29th with 24 students attending. IQTCUB has covered catering expenses with a total cost of 295 €.

Pictures corresponding to the "Introductory Course in Computational Chemistry" that took place on June 2012 at Chemistry Faculty of the *Universitat de Barcelona*.

d. *Advanced Course in Computational Chemistry.* Given the success of the first edition of the Introductory Courser un 2011 and the interest shown by students who participated, it has been decided to start a new course at a more advanced level with the main goal of improving previous knowledge in use of computers and, in particular, on Computational Chemistry. The course took place in July, 2nd-6th, 2012 and students attending being mainkly those who had participated in the first introductory course in 2011. The total cost of the course has been 295 € a corresponding to catering and have been taken from the IQTCUB budget.

Pictures corresponding to the “Advanced Course in Computational Chemistry” that took place on June 2012 at Chemistry Faculty of the *Universitat de Barcelona*.

II.2 IQTCUB SEMINARS AND CONFERENCES

Along 2012 a series of ten seminars have been organized by IQTCUB which are described below.

. **Prof. Juan Carlos Paniagua** (Universitat de Barcelona) Spain

Quantum theory: so true, so astonishing (1st part).

March 21st, 2012

2. **Prof. Juan Carlos Paniagua** (Universitat de Barcelona) Spain

Quantum theory: so true, so astonishing (2nd part).

March 28th, 2012

3. **Prof. Graeme Watson** (Trinity College Dublin) Irlanda

Solid State Modelling: from Catalysis to Semiconductors

April 11th, 2012

4. **Prof. Juan Carlos Paniagua** (Universitat de Barcelona) Spain

Quantum theory: so true, so astonishing (3rd part).

May 2nd, 2012

5. **Prof. Richard Catlow** (University College London) United Kingdom

Computational Studies of Catalytic and Energy Materials

May 17th, 2012

6. **Prof. Carlo Petrongolo** (University of Siena) Itàlia

Nonadiabatic Quantum Dynamics of Atom + Diatom Collisions

May 20th, 2012

7. **Prof. Fernando Martin** (Universidad Autónoma de Madrid) Spain

XUV/X-ray femto- and attosecond laser pulses for ultrafast electronic control in chemistry: towards attochemistry? And a new surface chemistry?

June 6th, 2012

8. **Prof. Juan Carlos Paniagua** (Universitat de Barcelona) Spain

   Quantum theory: so true, so astonishing (4th part).

   July 5th, 2012

9. **Prof. Vladimir Matolin** (Charles University in Prague) República Txeca

   Angle resolved resonance photoelectron spectroscopy: new tool of band mapping

   July 9th, 2012

10. **Prof. Marcel Swart** (Universitat de Girona) Spain

    Chemical reactivity of Endohedral Fullerenes

    October 17th, 2012

II.3 IQTCUB INVITED RESEARCHERS

Along 2012, a total of 16 researchers from all over the world have spent some time at the IQTCUB collaborating in different research projects.

1. **Prof. Andrey Belyaev** (invited visitor)
   Herzen University, St. Peterburg, Russia
   February-March 2012

2. **Darwin Burgos Carrasco** (invited visitor)
   Universidad de Chile, Chile
   February-June 2012

3. **Miroslava Nedyalkova** (HPCE visitor)
   University of Sofia, Bulgaria
   April-July 2012

4. **Zamaan Raza** (HPCE visitor)
   University College London, United Kingdom
   June-July 2012

5. **Dr. Laura Pitulice** (invited visitor)
   University West Timisoara, Romania
   June-September 2012

6. **Paul C. Jennings** (HPCE visitor)
   Universitat de Birmingham, United Kingdom
   July-September 2012

7. **Boutheina Kerkeni** (invited visitor)
   Observatoire de Meudon, Paris, France
   July-August 2012

8. **Sr. Patanachai Janthon** (invited visitor)
   Kasetsart University, Bangkok, Thailand
   July-December 2012

9. **Prof. Alexis Markovits** (HPCE visitor)

Université Pierre et Marie Curie, Paris, France
July-September 2012

10. **Prof. Silvia González** (invited visitor)
    Universidad Particular de Loja, Loja, Ecuador
    August-September 2012

11. **Dr. Stoyan Pisov** (HPCE visitor)
    University of Sofia, Bulgaria
    September 2012

12. **John Buckeridge** (HPCE visitor)
    University College London, United Kingdom
    October 2012

13. **Dave Gobrecht** (HPCE visitor)
    University of Basel, Switzerland
    October-November 2012

14. **Dr. Elizabeth Florez** (invited visitor)
    Universidad de Medellín, Colombia
    November 2012

15. **Maximiliano Porrini** (HPCE visitor)
    Edinburgh University, United Kingdom
    November 2012

16. **Dr. Noelia Faginas Lago** (invited visitor)
    Università di Perugia, Italy
    November 2012

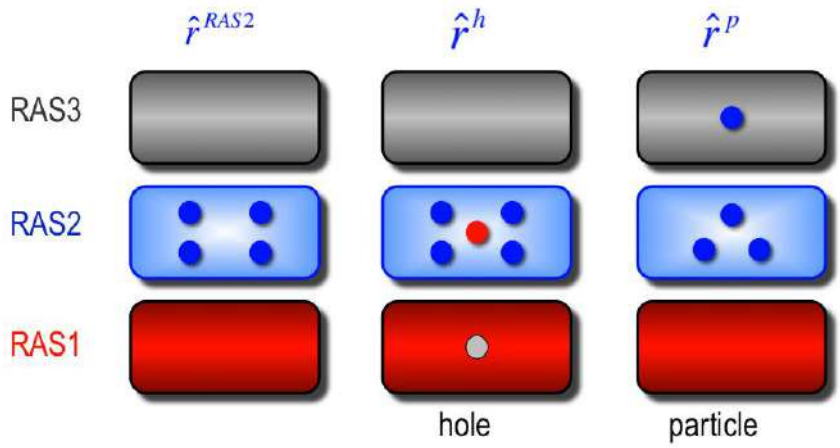
III. SCIENTIFIC ACTIVITY OF IQTCUB MEMBERS

III.1 HIGHLIGHTS FROM MOST RELEVANT RESULTS

Here some representative, relevant results are presented corresponding to each of IQTCUB the main research lines.

LINE 1. METHODS, ALGORITHMS AND COMPUTATIONAL TOOLS DEVELOPMENT

Avoided crossings, conical intersections, and low-lying excited states with a single reference method: The restricted active space spin-flip configuration interaction approach.
D. Casanova.
J. Chem. Phys., *137* (2012) 084105.



Schematic representation of the RAS-SF-CI wavefunction with up to one hole in RAS1 and one electron in RAS3.

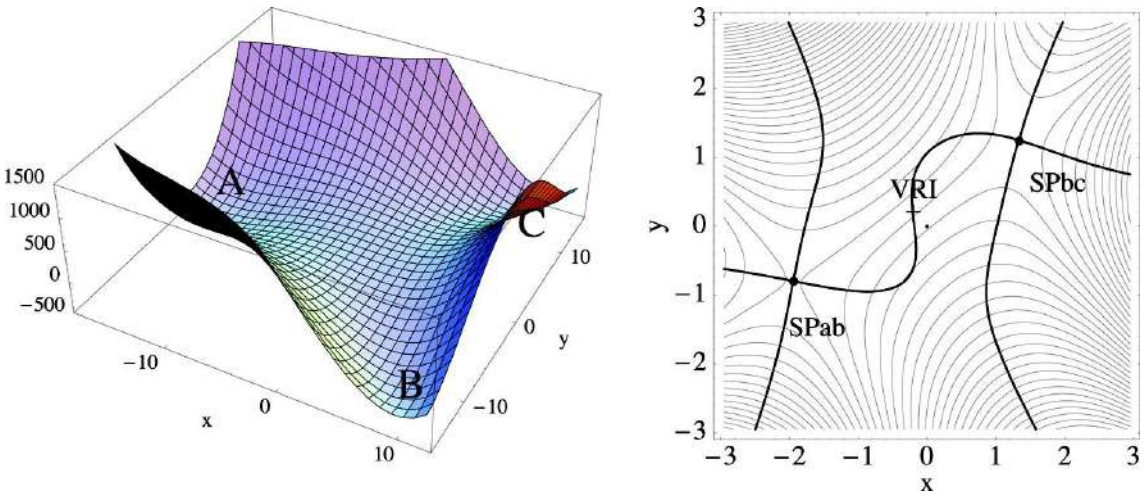
The restricted active space spin-flip CI (RASCI-SF) performance is tested in the electronic structure computation of the ground and the lowest electronically excited states in the presence of near-degeneracies. The feasibility of the method is demonstrated by analyzing the avoided crossing between the ionic and neutral singlet states of LiF along the molecular dissociation. The two potential energy surfaces (PESs) are explored by means of the energies of computed adiabatic and approximated diabatic states, dipole moments, and natural orbital electronic occupancies of both states. The RASCI-SF methodology is also used to study the

ground and first excited singlet surface crossing involved in the double bond isomerization of ethylene, as a model case. The two-dimensional PESs of the ground and excited states are calculated for the complete configuration space of torsion and pyramidalization molecular distortions. The parameters that define the state energetics in the vicinity of the conical intersection region are compared to CASSCF results. These examples show that it is possible to describe strongly correlated electronic states using a single reference methodology without the need to expand the wavefunction to high levels of collective excitations. Finally, RASCI is also examined in the electronic structure characterization of the ground and low-lying states of all-trans polyenes with two to seven double bonds and beyond. Transition energies are compared to TDDFT, CASSCF, and CASPT2 calculations, and to experimental data. The capability of RASCI-SF to describe the nature and properties of each electronic state is discussed in detail. This example is also used to expose the properties of different truncations of the RASCI wavefunction and to show the possibility to use an excitation operator with any number of α-to-β electronic promotions.

The Variational Structure of Gradient Extremals.

J.M. Bofill, W. Quapp, M. Caballero.

J. Chem. Theory Comput., *8* (2012) 927.



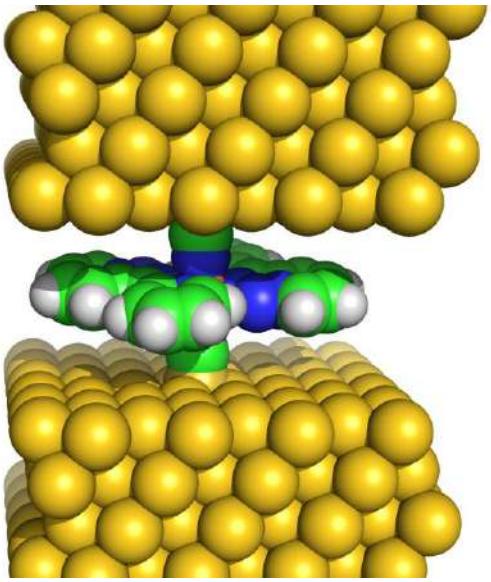
Left panel: PES associated to the mechanism of the reaction A → B + C. The mechanism for this reaction consists of two elementary reactions, namely, A → B and A → C. Each product is associated with different minimums in the PES. Right panel: GE in the enlarged center of the left panel. VRI: The valley from minimum B separates into two valleys over the SPs and a ridge between. The VRI point is crossed by the GE, whichconnects the two adjacent SPs.

LINE 2. COMPUTATIONAL MATERIALS SCIENCE

Coherent transport through spin-croosover single molecules.

D. Aravena, E. Ruiz.

J. Am. Chem. Soc., *134*, (2012) 777.

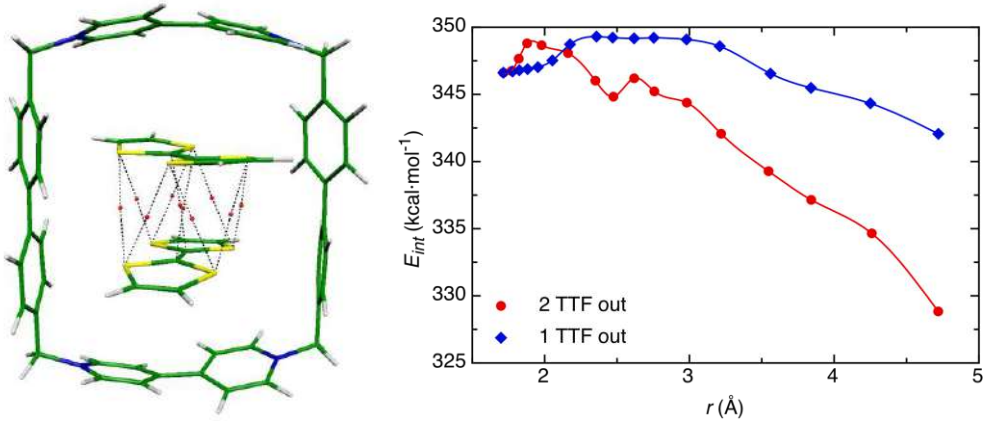


La tecnologia basada en silici està arribant al límit de grandària crítica, en què els efectes quàntics tenen un impacte sobre el correcte funcionament dels dispositius. Això ha empès els científics a concebre nous dispositius que aprofiten els fenòmens quàntics en el seu disseny. En aquest context, les molècules magnètiques han atret una considerable atenció degut al que algunes propietats d'aquests sistemes, com les transicions d'espín i els imans unimoleculars poden servir com a base per a nous dispositius de espintrònica molecular. Recentment hem presentat els resultats de càlculs DFT, combinats amb funcions de Green de no-equilibri, que permeten predir la resposta de corrent elèctric a un voltatge aplicat per a un dispositiu compost d'una molècula amb transició d'espín, *trans*-bis(isotiocianat) de ferro(II), connectat a dos elèctrodes d'or. Hem trobat que el corrent total depèn de l'estat d'espín de la molècula. Aquesta propietat està relacionada amb l'energia dels orbitals d en el centre Fe^{II} en ambdós estats d'espín i mostra que la conductància està profundament lligada al reordenament electrònic que dóna lloc a la transició d'espín. En el cas de la molècula d'espín alt, també hem trobat que el corrent té un caràcter de spin polaritzat, amb la major part de la conductància deguda als electrons β, comportant-se com un dispositiu de filtre d'espín. Aquest resultat també està lligat al desdoblament del orbitals d del catió Fe^{II} i ha de ser una característica general dels dispositius basats en complexes de Fe^{II} amb transició d'espín.

The Nature of the [TTF]·+⋯ [TTF]·+ Interactions in the [TTF]22+ Dimers Embedded in Charged [3]Catenanes: Room-Temperature Multicenter Long Bonds.

M. Capdevila-Cortada, J.J. Novoa.

Chem. Eur. J., *18* (2012) 5335.

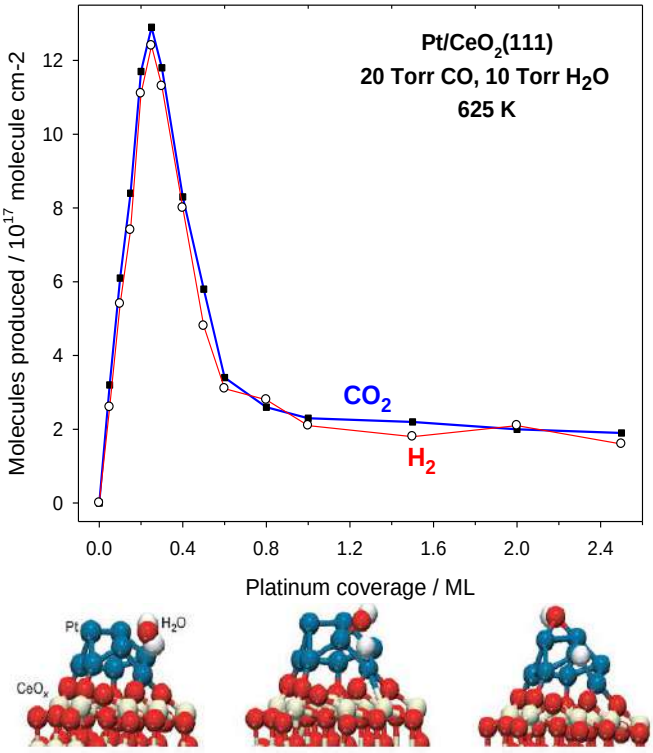


Due to the high impact of a recent *Nature Chemistry* publication where diamagnetic $[TTF]_2^{2+}$ dication dimers were obtained at room temperature by means of synthesizing a *[3]catenane* supramolecular entity, in this work we show an exhaustive theoretical study revealing the nature of its interactions and the stabilization of the $[TTF]_2^{2+}$ dimer dication within the supramolecular entity. By means of DFT calculations the aforementioned *[3]catenane*$^{m+}$ and the inclusion complex $([TTF]_2^{n+}$ C $CBPQT^{4+})^{m+}$, where CBPQT is the central macrocycle of the [3]catenane, in their different oxidation states where studied in the gas phase, solution, and solid state. Our results show the stabilization that the $[TTF]^{n+}$ moieties experience when they are part of the *[3]catenane*, although these would not be high enough to form a $[TTF]_2^{2+}$ dication dimer in the gas phase. On the contrary, when solvent or counterions are taken into account the whole system becomes stable. Despite the fact that this instability *per se* in the gase phase would make the *[3]catenane* dissociate, it does not since it would mean a covalent bond breaking.

A New type of Strong Metal-Support Interaction and the Production of H_2 through the Transformation of Water on $Pt/CeO_2(111)$ and $Pt/CeO_x/TiO_2(110)$ catalysts.

A. Bruix, J. A. Rodriguez, P. J. Ramírez, S. D. Senanayake, J. Evans, J. B. Park, D. Stacchiola, P. Liu, J. Hrbek, F. Illas

J. Am. Chem. Soc., *134* (2012) 8968.



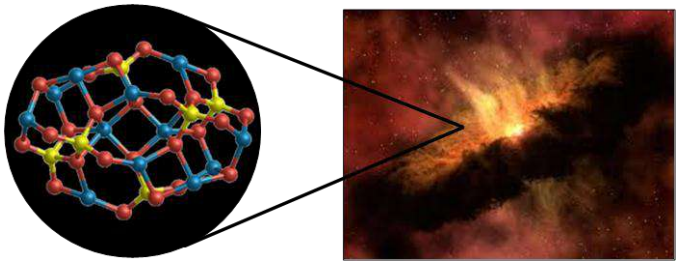
Experimental values of hydrogen production through the water gas shift (WGS) reaction catalyzed by Pt nanoparticles supported on CeO2 as a function of the particle size in the Pt/CeO2 catalys and model used to explain the observed phenomenon.

The WGS reaction, $CO + H_2O \rightarrow CO_2 + H_2$, is used in industry to remove the CO produced in hydrocarbon steam reforming which is the main source of molecular hydrogen. The small amount of CO left in the gas stream poisons the catalysts used in subsequent processes such as hydrotreatment to remove S from oil in the refineries before entering cracking or in the fuell cells. In this work, experiments show that the reactivity of Pt nanoparticles supported on CeO_2 changes dramatically with particles size. The theoretical models and computational work carried out by IQTCUB researchers show that the origin of this behavior is a new specific support effect which, in this way, participates directly in the chemical reaction. This effect has been highlighted by Prof. C. T. Campbell in a note recently published in *Nature Chemistry* 4 (2012) 597.

Efficient nucleation of stardust silicates via heteromolecular homogeneous condensation.

F. Goumans, S.T. Bromley.

Mon. Not. R. Astron. Soc., *420* (2012) 3344.

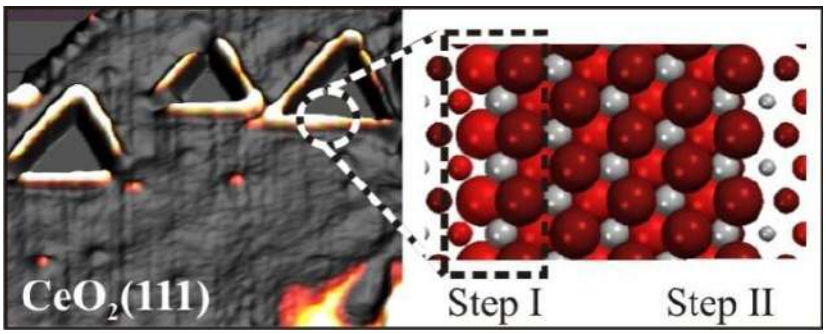


An atomically detailed viable route to circumstellar dust nucleation is reported for the first time, based on global optimisation and *ab inito calculations*.

Formation of one-dimensional electronic states along the step edges of CeO_2(111)

N. Nilius, S.M. Kozlov, J.-F. Jerratsch, M. Baron, X. Shao, F. Viñes, S. Shaikhutdinov, K.M. Neyman, H.-J. Freund.

ACS Nano, *6* (2012) 1126.



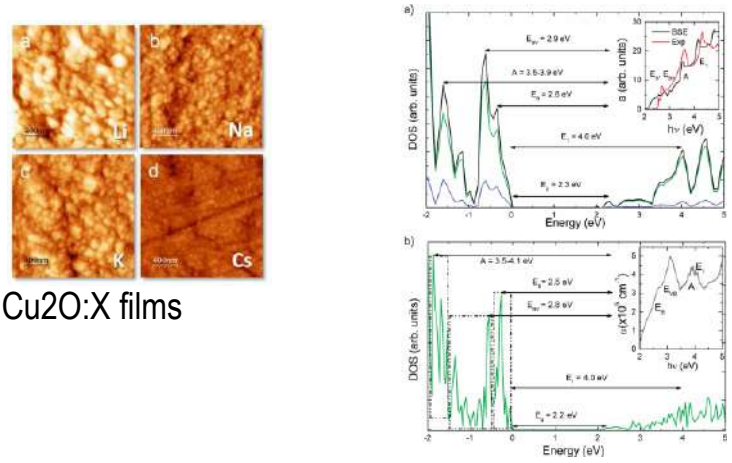
Outstanding red-ox properties of cerium oxide attract worldwide attention to this material as a catalyst or a catalyst support. In the above mentioned paper we have shown that some properties of ceria surfaces may be altered by high-temperature annealing, which would induce formation of ceria nanoislands bordered by three different step types with different properties. The paper is devoted to determination of atomic structure of these steps and characterization of their electronic structure using scanning tunneling microscopy and spectroscopy experiments combined with computational methods based on density functional theory. The results of theoretical and experimental investigations nicely agreeing with each other reveal that properties

of steps are strongly affected by dipole moments produced by missing O anions. This work paves the way for further theoretical and experimental studies on model ceria catalysts with well characterized nanostructure

Disruption of the Chemical Environment and Electronic Structure in p-Type Cu2O Films by Alkaline Doping

F. Caballero-Briones, A. Palacios-Padros, O. Calzadilla, I. de P. R. Moreira, F. Sanz,

J. Phys. Chem. C *116* (2012) 13524



Left: topographic AFM images (2 × 2 μm^2) showing the surface morphology of Cu_2O films doped with (a) Li, (b) Na, (c) K and (d) Cs. Notice the reduction in grain size from Li to Cs doped materials. Right: Calculated electronic density of states for (a) Cu_2O and (b) Cu_2O:K. A rigid band model has been used to interpret the nature of the states defining Eg as well as the EB, EBV, A, and E1 peaks observed in the corresponding absorption spectra.

This work is a collaboration with the Bioelectrochemistry and Nanotechnology group leaded by Prof. F. Sanz. Here we describe and analyze the interesting properties of Cu_2O films doped with alkaline ions (Li^+, Na^+, K^+ and Cs^+) prepared by Cu anodization. The main effects of the alkaline doping on the optical properties were a reduction in the direct band gap and an approach of the acceptor level edge to the maximum of the valence band, which induce important changes in the observed optical response. First principles band structure calculations on models for the alkaline doped Cu_2O systems suggest that the main effect of the alkaline substitution of copper atoms consists in polarizing the O states, which causes a reduction in the insulating gap and splitting of the density of states just below the Fermi level. The nature of the oxygen-dopant interaction was attractive for Li, slightly repulsive for Na and clearly repulsive for K and Cs. This fact provides an explanation for the observed surface accumulation of K^+ and Cs^+ that hinders vacancy diffusion and blocks film growth, leading to a reduction of roughness and thickness of

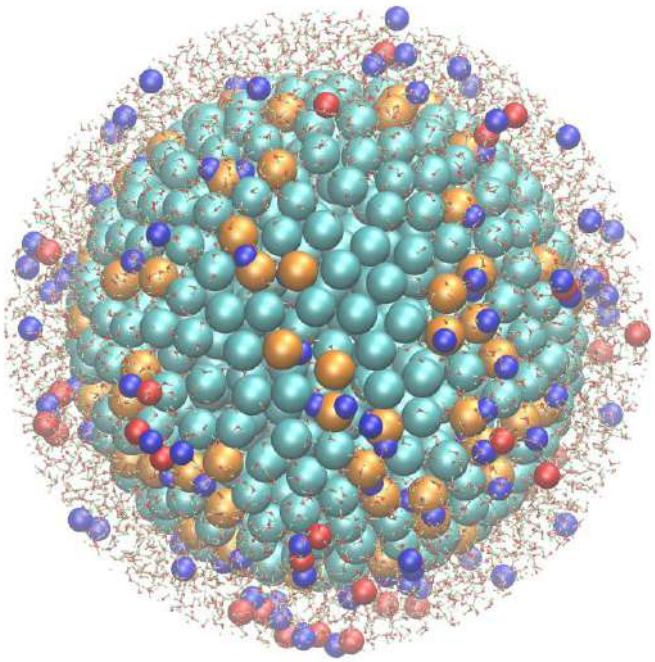
crystallites as the ion size increases.

LINE 3. COMPUTATIONAL BIOCHEMISTRY AND *SOFT MATTER*

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

M. Nedyalkova, S. Madurga, S. Pisov, I. Pastor, E. Vilaseca, F. Mas.

J. Chem. Phys., *137* (2012) 174701.



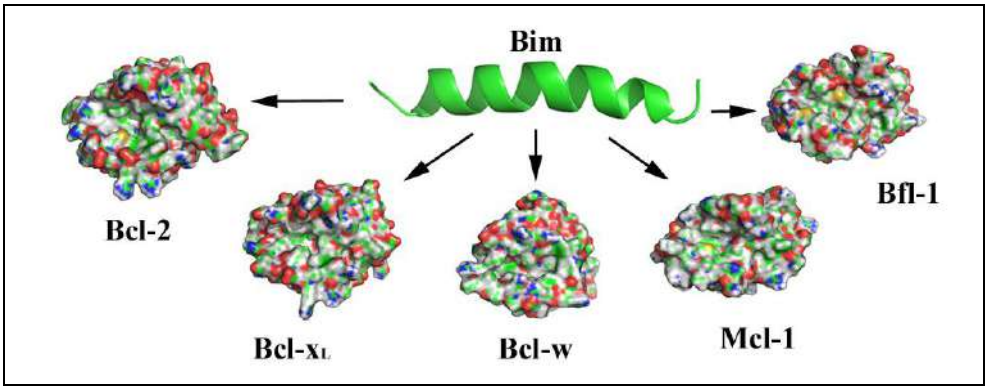
Snapshot of a simulation of the −100e charged nanoparticle in 1 M NaCl solution. Only water molecules, Na^+ ions (in blue), and Cl^- ions (in red) close to 1.0 nm from the nanoparticle surface are displayed.

Molecular dynamics simulations were performed to study the ion and water distribution around a spherical charged nanoparticle. A soft nanoparticle model was designed using a set of hydrophobic interaction sites distributed in six concentric spherical layers. In order to simulate the effect of charged functionalyzed groups on the nanoparticle surface, a set of charged sites were distributed in the outer layer. Four charged nanoparticle models were studied in NaCl and $CaCl_2$ salt solutions at 1 M and 0.1 M concentrations to evaluate the effect of the surface charge, counterion valence, and concentration of added salt. We obtain that Na^+ and Ca^{2+} ions enter inside the soft nanoparticle. Monovalent ions are more accumulated inside the nanoparticle surface.

Molecular Determinants of Bim(BH3) Peptide Binding to Pro-Survival Proteins.

L. Delgado-Soler, M. Pinto, K. Tanaka-Gil , J. Rubio-Martinez.

J. Chem. Inf. Model., *52* (2012) 2107.



The Bcl-2 family proteins are well-characterized regulators of the intrinsic apoptotic pathway. Proteins within this family can be classified as either prosurvival or prodeath members. The balance between them present at the mitochondrial membrane is what determines if the cell lives or dies. For this reason, the design of small molecules inhibiting the proapoptotic proteins has emerged as a promising therapeutic strategy for cancer treatment during the last years. Although the precise mechanism by which this family of proteins regulates apoptosis is still poorly understood, it is well accepted that anti- and proapoptotic proteins modulate their opposite functions through heterodimerization. The experimental structures of antiapoptotic proteins complexed with peptides derived from the BH3 domain of proapoptotic proteins has provided the first insights into the molecular mechanism of the heterodimerization of this family of proteins. In these complexes, the antiapoptotic protein forms a hydrophobic cleft on its surface wherein the hydrophobic face of an amphipathic α-helix containing the BH3 domain of the proapoptotic protein binds. In this scenario, it was postulated that small molecules mimicking the BH3 α-helix of proapoptotic proteins may be able to bind to the same hydrophobic groove of antiapoptotic Bcl-2 family members blocking their heterodimerization and leading to apoptosis. One of the most important considerations to bear in mind when designing BH3 mimetics is the different affinity of BH3 domains for individual antiapoptotic proteins. Bim and Puma are the only proapoptotic proteins that bind to all pro-survival proteins with similar affinities. Thus, mimetics of any of these proteins should be able to bind to all the antiapoptotic proteins and should represent a first step in

the development of new anticancer agents.

The reaction coordinate of a bacterial GH47 α-mannosidase: a combined quantum mechanical and structural approach.

A. J. Thompson, J. Dabin, J. Iglesias-Fernández, A. Ardèvol, Z. Dinev, S. J. Williams, O. Bande, A. Siriwardena, C. Moreland, T.-C. Hu, D. K. Smith, H. J. Gilbert, **C. Rovira***, G. J. Davies*.

Angew. Chem. Int. Ed. *51* (2012) 10997-11001. Selected as Very Important Paper (VIP, top 5% of the journal). Inside back cover.

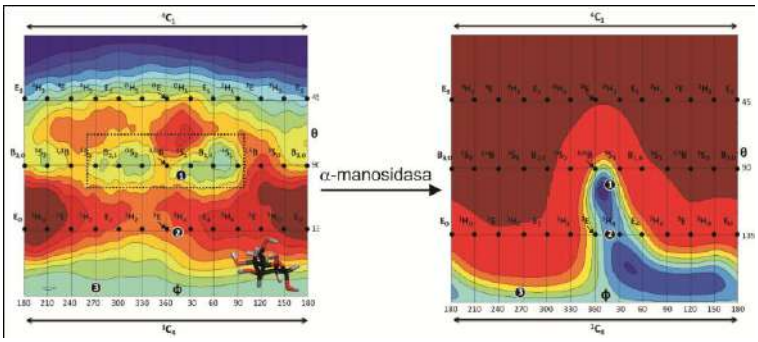


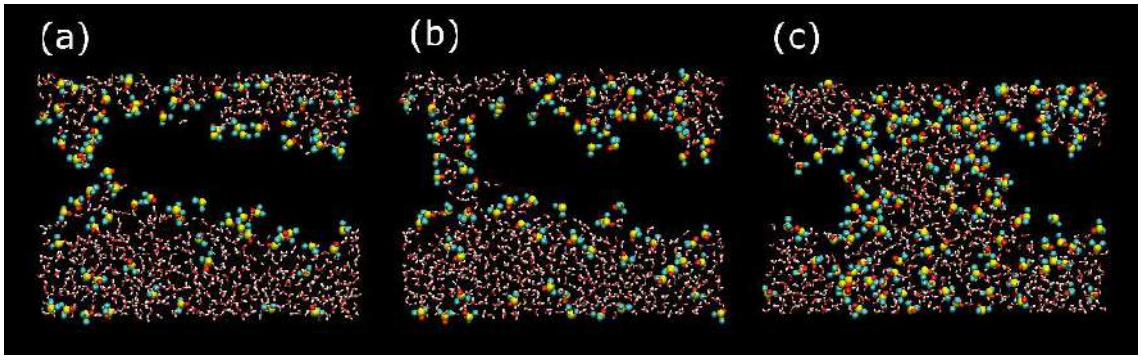
Figure. Conformational space reduction of a mannose unit by the α-manosidase enzyme, as well as its conformational itinerary during the chemical reaction.

α-manosidase enzymes are responsible of trimming and/or remodeling certain carbohydrates that are covalently attached to proteins. Alteration, excess and deficiency of these carbohydrates lead to diseases such as some tumors or the so-called lysosomal diseases. Starting from the structure of the carbohydrate-enzyme complex, determined at atomic resolution, and using *ab initio* molecular dynamics-based methods (in particular, QM/MM metadynamics) we demonstrated that the enzyme drastically alters the conformational landscape of the carbohydrate with respect to the one of the isolated carbohydrate. Interestingly, the conformations that "survive" are the ones that the carbohydrate adopts during the catalytic reaction. Therefore, the enzyme imposes the conformations that favor catalysis

Effects of Dymethyl Sulfoxide in Cholesterol-Containing Lipid Membranes: A Comparative Study of Exeriments In Silico and with Cells.

M-A. de Ménorval, LL.M. Mir, M.L. Fernández, R. Reigada.

PLoS One, *7* (2012) e41733.



Pore formation in a lipid membrane due to the effect of Dimethyl Sulfoxide

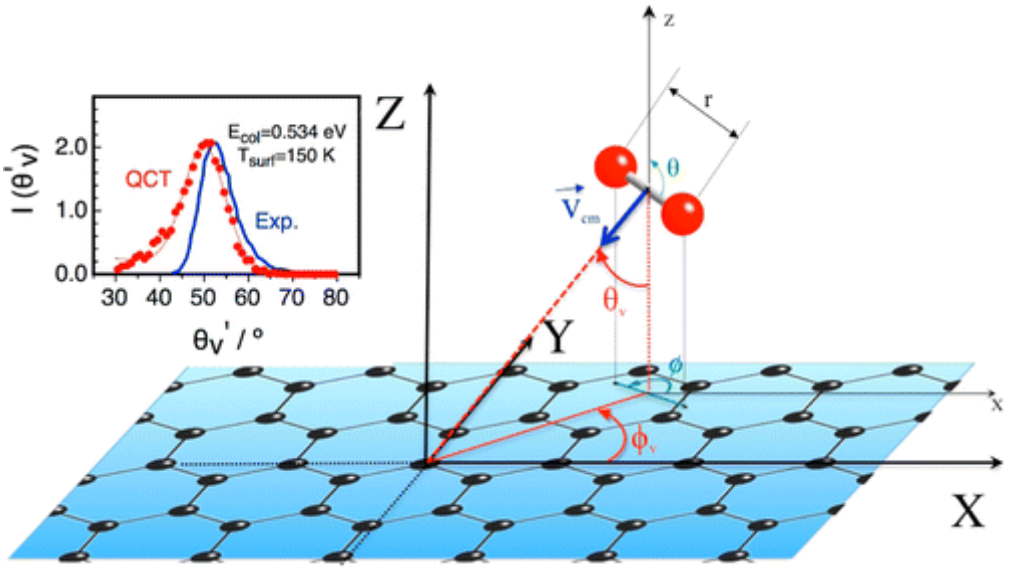
We use Molecular Dynamics simulations and in vivo experiments to study the effect of dimethyl sulfoxide (DMSO) in lipid membranes. Three modes of action of DMSO are identified in both numerical simulations and experimental observations. At low concentrations, membrane fluctuations are promoted, at moderate concentrations, stable membrane pores are formed, and at large concentrations, membrane collapses. Simulations have unveiled the molecular mechanisms of these three mdoes of action, and experiments have confirmed their existence in cellular systems. The relevance of this work is related to the importance of pore formation in the electroporation techniques used in electrochemotherapy treatments. The experiments have been conducted by the research group of Dr. Mir, pioneer in electrochemotherapies, and our results open new possibilities to use DMSO that could improve these treatments.

LINE 4. REACTIVITY AND REACTIONS DYNAMICS

Dynamics of the oxygen molecules scattered from graphite (0001) surface and comparison with experimental data.

V. Morón, L. Martin-Gondre, P. Gamallo, R. Sayós.

J. Phys. Chem. C *116* (2012) 21482.



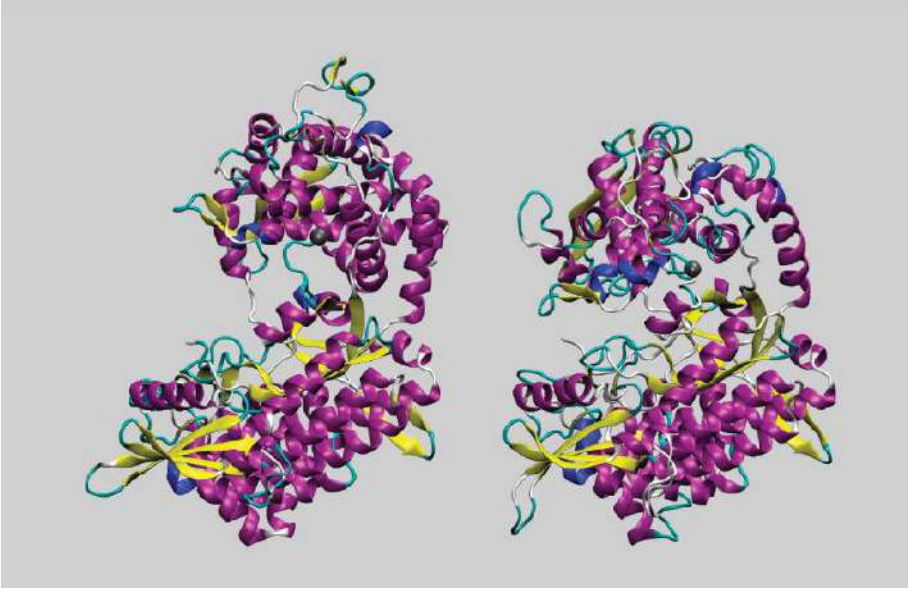
A quasiclassical trajectory dynamics study of molecular oxygen colliding over a free of defects and clean graphite (0001) surface has been performed with a recently published density functional theory based flexible periodic London-Eyring-Polanyi-Sato potential energy surface (PES). Although the PES was mainly constructed for describing accurately the recombination of atomic oxygen (Eley-Rideal reaction) over an O-preadsorbed surface, here we show that this PES is also reliable to study the scattering of O_2 over graphite surface. Thus, several initial conditions have been explored: collision energies ($0.2 \leq E_{col} \leq 1.2$ eV), incident angles ($\theta_v = 0°$, 45°), surface temperatures ($100 \leq T_{surf} \leq 900$ K) and some rovibrational O_2 levels (v = 0,1,2 and j = 1,17,25). The calculated polar scattering angular distributions are in good agreement with the experimental ones in a wide range of explored conditions. Moreover, the comparison with hyperthermal experimental data (i.e., $<E_{col}>=10.46$ eV), T_{surf} = 503 K, v=0, j=1 and θ_v = 45°),

which was unclear in a previous work, has been finally clarified. The effect of O_2 (v,j) internal state on the scattering is very small.

The Large Scale Conformational Change of the Human DPP III–Substrate Prefers the "Closed" Form.

A. Tomić, M. González, S. Tomić.

J. Chem. Inf. Model., *52* (2012) 1583.



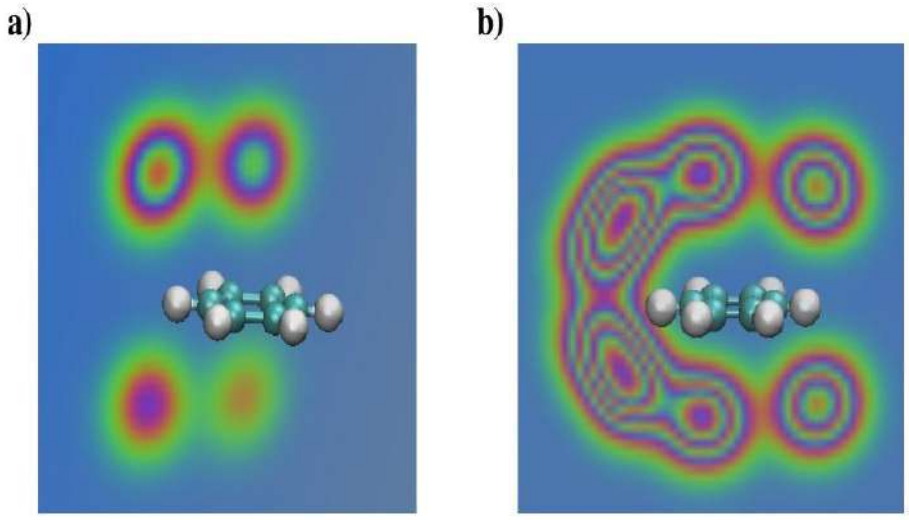
Initial structure of DPP III (left) and structure obtained after 101 ns of MD simulation (right).

The wide space available between the two domains and the broad substrate specificity that presents the human variant of the dipeptidil peptidase III (DPP III) enzyme suggests that it may experience significant conformational changes. And indeed this is what has been observed in Molecular Dynamics (MD) simulations (> 100 ns), and free energy calculations show that the preferred synthetic substrate (Arg-Arg-2-naphtylamide) has a stronger binding to the enzyme in the "closed" conformation than in the "open" one. Our assumption that the Asp372 residue plays a crucial role in the interdomain closing was evidenced by MD simulations on the Asp372Ala variant. According to the MM-PBSA calculations, the electrostatic component of the solvation free energy is found to be larger for the protein in its closed form than for the less compact form. However, the gain in entropy caused by the water molecules released from the interdomain space balances this negative effect. So, we have a very interesting process which is driven by the increase of entropy, in accordance with what has been suggested very recently by the experiments.

Competitive Role of CH_4-CH_4 and CH-π interactions in the C_6H_6–$(CH_4)_n$ aggregates: The transition from dimmers to cluster features.

M. Albertí, A. Aguilar, J.M. Lucas, F. Pirani.

J. Phys. Chem. A, *116* (2012) 5480.



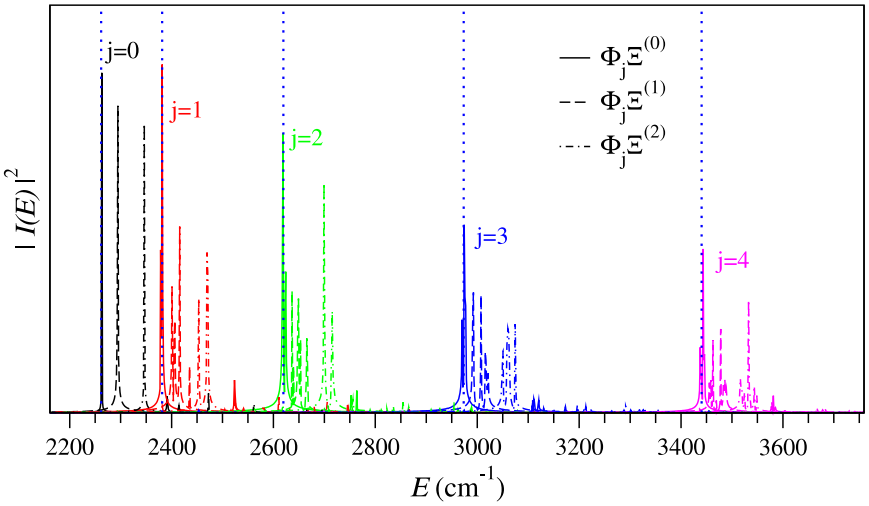
Two-dimensional maps of the probability density of the CH_4 molecules around benzene.

The formulation of both the CH4-CH4 and the CH4-Benzene (CH4-Bz) intermolecular interactions has been applied to investigate some macroscopic properties of methane and to analyze the spatial distribution of the methane molecules around Bz. It has been observed that different stable isomers of some small systems (containing only few methane molecules) have similar energies, allowing frequent interconversions between isomers even at very low temperatures. However, a preferential tendency of the methane molecules to occupy axial positions around Bz has been observed, as shown on the left and on the right hand side panels of the figure for the Bz-(CH4)3 and Bz-(CH4)7, respectively.

Hydrogen confined in single-wall carbon nanotubes: Anisotropy effects on ro-vibrational quantum levels.

J. Suárez, F. Huarte-Larrañaga.

J. Chem. Phys. *137* (2012) 064320.



Energy spectrum pf the H_2 molecule in the ground vibrational state and confined in a carbon nanotube of chirality (8,0). Different colored lines correspond to different rotational states.

This article presents the quantum dynamics study in which we obtained the energy levels of the hydrogen molecule encapsulated in the inner cavity of a single walled carbon nanotube. The effects of confinement in nanostructures have awakened a great amount of interest in the recent past. In addition to this, carbon nanotubes have shown an outstanding capability to encapsulate molecules in nearly monodimensional environments and this feature could be important in processes such as hydrogen physisorption. The simulations we have carried out include explicitly all degrees of freedom of the confined molecule, revealing how vibrational motion is affected by the confining potential generated by the walls of the nanostructures. Previous works that neglected this degree of freedom did not observe this feature. However, the most important effects are the molecule rotation and the appearance of a quantized translational motion. We have also analyzed the dependence of the confinement effects on the interaction potential by tuning the different parameters in the empirical carbon-hydrogen potential.

III.2 PUBLICATION LIST

The list below includes articles published during 2012 and those of 2011 which were not included in the 2011 Memoir since they were published after completion of that document.

ARTICLES

1. *Conformational analyses of the reaction coordinate of glycosidases.*
   G. J. Davies, A. Planas, C. Rovira.
   Acc. Chem. Res. *45* (2012) 308.

2. *Formation of one-dimensional electronic states along the step edges of CeO_2(111).*
   N. Nilius, S.M. Kozlov, J.-F. Jerratsch, M. Baron, X. Shao, F. Viñes, S. Shaikhutdinov, K.M. Neyman, H.J. Freund.
   ACS Nano *6* (2012) 1126.

3. *Chemistry: A Panoply of Arrows.*
   S. Alvarez.
   Angew. Chem. Int. Ed. *51* (2012) 590.

4. *The reaction coordinate of a bacterial GH47 α-mannosidase: a combined quantum mechanical and structural approach.*
   A. J. Thompson, J. Dabin, J. Iglesias-Fernández, A. Ardèvol, Z. Dinev, S. J. Williams, O. Bande, A. Siriwardena, C. Moreland, T.C. Hu, D. K. Smith, H. J. Gilbert, C. Rovira, G. J. Davies.
   Angew. Chem. Int. Ed. *51* (2012) 10997.

5. *The reaction mechanisms of heme catalases: An atomistic view by ab initio molecular dynamics.*
   M. Alfonso-Prieto, P. Vidossich, C. Rovira.
   Arch. Biochem. Biophys. *525* (2012) 121.

6. *Size-controlled nanopores in lipid membranes with stabilizing electric fields.*
   M.L. Fernández, M. Risk, R. Reigada, P.T. Vernier.
   Biochem. Biophys. Res. Comm. *423* (2012) 325.

7. *On the Interaction of Polycyclic Aromatic Compounds with Graphene.*
   S.M. Kozlov, F. Viñes, A. Görling.
   Carbon *50* (2012) 2482.

8. *Human and rodent aldo-keto reductases from the AKR1B subfamily and their specificity with retinaldehyde.*
   F. X. Ruiz, A. Moro, O. Gallego, A. Ardèvol, C. Rovira, J. M. Petrash, X. Parés, J. Farrés.
   Chem. Biol. Interact. *19* (2011) 199.

9. *Evidence for atomic mixing via multiple intermediates during the dynamic interconversion of silicate oligomers in solution.*
K. Jelfs, E. Flikkema, S. T. Bromley .
Chem. Commun. *48* (2012) 46.

10. *Octahedrality versus tetrahedrality in stoichiometric ceria nanoparticles.*
A. Migani, K. Neyman, S. T. Bromley.
Chem. Commun. *48* (2012) 4199.

11. *Enhanced bistability by guest inclusion in Fe(II) spin crossover porous coordination polymers.*
F. J. Muñoz Lara, A. B. Gaspar, D. Aravena, E. Ruiz, M. C. Muñoz, M. Ohba, R. Ohtani, S. Kitagawa, J. A. Real.
Chem. Commun. *48* (2012) 4686.

12. *Field and dilution effects on the slow relaxation of a luminescent DyO_9 low-symmetry single-ion magnet.*
J. Ruiz, A. J. Mota, A. Rodríguez-Diéguez, S. Titos, J. M. Herrera, E. Ruiz, E. Cremades, J. P. Costes, E. Colacio.
Chem. Commun. *48* (2012) 7916.

13. *Electronic structure and symmetry in conjugated π-electron systems.*
P. Alemany, D. Casanova, C. Dryzun.
Chem. Eur. J. *17* (2011) 14896.

14. *Triangular Nickel Complexes Derived from 2-Pyridylcyanoxime: An Approach to the Magnetic Properties of the $[Ni_3(\mu_3\text{-}OH)\{pyC(R)NO\}_3]^{2+}$ Core.*
J. Esteban, E. Ruiz, M. Font-Bardia, T. Calvet, A. Escuer.
Chem. Eu. J. *18* (2012) 3637.

15. *The Nature of the $[TTF]^{\bullet+}\cdots[TTF]^{\bullet+}$ Interactions in the $[TTF]_2^{2+}$ Dimers Embedded in Charged [3]Catenanes: Room-Temperature Multicenter Long Bonds.*
M. Capdevila-Cortada, J.J. Novoa.
Chem. Eur. J *18* (2012) 5335.

16. *The structural Diversity Triggered by Intermolecular Interactions between Au^IS_2 groups: Aurophilia and Beyond.*
M.-R. Azani, O. Castillo, M. L. Gallego, T. Parella, G. Aullón, O. Crespo, A. Laguna, S Alvarez, R. Mas-Ballesté, F. Zamora.
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2. *Potential energy surfaces for the dynamics of elementary gas-surface processes.*
   P. Gamallo, L. Martin-Gondre, R. Sayós, C. Crespos, P. Larregaray.
   Dynamics of gas-surface interactions: atomic-level understanding of scattering processes at surfaces (2012) (Springer-Verlag, in press).

3. *Molecular dynamics study of hydrogen atom recombination over silica, based on a new analytical DFT potential energy surface*
   P. Gamallo , M. Rutigliano , S. Orlandini , M. Cacciatore, R. Sayós.
   Proceedings of the 28th International Symposium on Rarefied Gas Dynamics.
   AIP Conference Proceedings (July, 2012) (in press).

4. *Assaig sobre una manera de determinar les masses relatives de les molècules elementals dels cossos, així com de les proporcions amb què entren en aquests compostos, d'Amedeo Avogadro.*
   Xavier Giménez, Pere Alemany.
   Clàssics de la Química *6* (2012) (Societat Catalana de Química, Barcelona) .

5. *Les sortides de camp com a recurs en educació química: itinerari ambiental de Castellciuró a Santa Creu d'Olorda.*
   Francesc Centellas, Montserrat Inglés, Laura Rosell, Enric Brillas, Robert Cruañas, Montserrat Cruells i Xavier Giménez.
   IV Jornades sobre l'Ensenyament de la Química, Societat Catalana de Química. Barcelona, 2012.

6. *Dynamics of Alkali Ions-Neutral Molecules Reactions: Radio Frequency-Guided Beam Experimental Cross-Sections and direct Quasiclassical Trajectory Studies.*
   J. Aguilar, J. de Andrés, J.M. Lucas, M. Albertí, F. Huarte-Larrañaga, D. Bassi and A. Aguilar.
   28th International Symposium on Rarefied Gas Dynamics, M. Mareschal and A. Santos, eds. (**AIP Conference Proceedings**, Melville, NY, 2013)

III.3 OTHER ACTIVITIES

DOCTORALS THESES 2012

1. *Propietats magnètiques i transport quàntic en imants unimoleculars: Un estudi teòric.*
   Eduard Cremades Martí
   Facultat de Química, Universitat de Barcelona.
   Gener 2012.

2. *Study of molecular mechanisms in glycoside hydrolases and transferases by ab initio molecular dynamics.*
   Albert Ardèvol Grau
   Facultat de Ciències, Universitat Autònoma de Barcelona.
   Gener 2012.

3. *QM/MM investigation of the reaction mechanism of the NS3/NS4A hepatitis C protease with its main substrates.*
   Alejandro Rodríguez García
   Facultat de Química, Universitat de Barcelona.
   Abril 2012.

4. *Aplicació i desenvolupament de mètodes mecano- quàntics multiconfiguracionals per a l'estudi de reaccions químiques.*
   Marc Moix Teixidor
   Facultat de Química, Universitat de Barcelona.
   Octubre 2012.

5. *Medidas de forma y simetría en compuestos con número de coordinación elevados y clústeres de alta nuclearidad.*
   Antonio Ruiz Martínez
   Facultat de Química, Universitat de Barcelona.
   Novembre 2012.

6. *Active e-learning and a distributed computing approach to the simulation of chemical reactions.*

   Osvaldo Gervasi

   Facultat de Química, Universitat de Barcelona.

   Novembre 2012.

7. *Complejación y activación de moléculas diatómicas en sistemas biomiméticos.*

   Benjamin Peigné

   Facultat de Química, Universitat de Barcelona.

   Novembre 2012.

MASTERS THESES 2012

1. *Estudio teórico de la formación de dímeros derivados del TTF en clips moleculares a temperatura ambiente.*

   Maria Fumanal Quintana

   Facultat de Química, Universitat de Barcelona.

   Setembre 2012.

2. *Química Teórica y Computacional y Estudio Monte Carlo de la difusión 2D en medios densos.*

   Santiago Alonso Gil

   Facultat de Química, Universitat de Barcelona.

   Setembre 2012.

SCIENTIFIC CONFERENCES AND MEETINGS 2012

2nd International Symposium on Intermetallic Compounds in Methanol Steam Reforming
Munich (Germany)

First-principles modelling of catalytically relevant surface alloys: PdAg, PdAu and AuAg (Oral)
K.M. Neyman

Arrangement of components in intermetallic PdZn films on Pd(111) modified by CO adsorption (Oral)
S.M. Kozlov, C. Weilach, G. Rupprechter, K.M. Neyman

Structure and stability of PdAu bimetallic nanocrystallites under hydrogenation conditions: A DFT study (Oral)
I.V. Yudanov, K.M. Neyman

5th International Conference on Molecular Materials (MOLMAT)
Barcelona (Spain)

A Novel Metal-free Full Organic Magnet (Poster)
S. Latorre, I. de P. R. Moreira, J. M. Bofill, F. López-Calahorra

Study of magneto-structural correlations of ferromagnetic triply heterobridged dinuclear copper(II) compounds" (Poster)
R. Costa, I. de P. R. Moreira, F. Illas, N. Wannarit, C. Pakawatchai, S. Youngme

Stereochemical Analysis of Coordination Spheres with Shape 2.0 (Oral)
S. Alvarez

7th International Conference on Surfaces, Coatings and Nanostructured Materials (NANOSMAT)
Prague (Czech Republic)

Alkaline Doping Causes Disruption Through the Chemical Environment and Electronic Structure in Anodic p-Type Cu2O Films (Poster)
F. Caballero-Briones, A. Palacios-Padrós, O. Calzadilla, I. de P. R. Moreira, F. Sanz

8th Congress on Electronic Structure: Principles and Applications (ESPA 2012)
Barcelona (Spain)

Chair
J.J. Novoa

Scientific Comittee
F. Illas, J.J. Novoa, S. Álvarez

Organizing Commitee
C. Sousa, I. de P. R. Moreira, R. Sayós, F. Mota, M. Deumal, J. Ribas, M. Capdevila, S.

Vela, A. Bruix

Photocycle of the light-induced spin-crossover process in the $[Fe(bpy)_3]^{2+}$ complex (Poster)
C. Sousa

Exchange Coupling in Chalcopyrite ($CuFeS_2$): A DFT+U Study (Poster)
S. Conejeros, P. Alemany, M. Llunell, I. de P. R. Moreira

Synthesis of new molecules without metallic atoms with magnetic properties (Poster)
C. Heras, S. Latorre, F. López-Calahorra, J. M. Bofill, I. de P. R. Moreira

Quasiclassical trajectory dynamics study of O/O_2 collisions over a clean/O-preadsorbed graphite (0001) surface with a new FPLEPS potential energy surface
P. Gamallo, V. Morón, L. Martin-Gondre, R. Sayós

Nature of the electronic correlation in DFT (Poster)
M. Caballero, J. M. Bofill, I. de P. R. Moreira

Interaction of metal on son gold surfaces
M. Nedyalkova, S. Madurga, S. Pisov, e. Vilaseca, F. Mas

Molecular Dynamics Simulation and Free Energy Calculation Studies of the Binding Mechanism of Inhibitors with B-Raf Kinase
Coronel Luis, Granadino-Roldán José Manuel, Tomás M. Santos, Pujol Maria Dolors, Rubio-Martinez Jaime

Towards the design of A Proliferation-Inducing Ligand (APRIL) inhibitors.
González-Mendióroz Maite, Álvarez-Vázquez Ana Belén, Planelles-Carazo Lourdes, Jaime Rubio-Martinez

Computation and rationalization of the photophysical properties of Ir(III) complexes as triplet emitters (Poster)
C. Climent, D. Casanova , P. Alemany , P. Alam, I. R. Laskar

A Continuous Symmetry Measures Analysis of the Electronic Structure in non Planar Conjugated Hydrocarbons (Poster)
P. Alemany, M. Llunell, A. Carreras y D. Casanova

Reactive processes in gas phase $i\text{-}C_3H_7Cl + Na^+$ collisions. An experimental and theoretical comparison (Poster)
J. Aguilar, J.M. Lucas, J. de Andrés, F. Huarte-Larrañaga, M. Albertí, A. Aguilar

8th International Workshop on Oxide Surfaces (IWOX-VIII)
Baqueira-Beret (Spain)

Modeling and understanding structure and reactivity of ceria well defined surfaces and nanoparticles (Invited Lecture)
F. Illas

11th Greta Pifat-Mrzljak International School of Biophysics
Primosten (Croatia)

The reaction of the hepatitis C virus NS3/NS4A protease with its main substrate. A QM/MM investigation
J.A. Martínez, R. Martínez, M.P. Puyuelo, L. Masgrau, M. González

13-th V.A. Fock Meeting on Quantum and Computational Chemistry
Astana (Kazajstan)

Continuous Symmetry Measures: Definition and Applications in Theoretical Chemistry
P. Alemany

14th International Congress of Quantum Chemistry
Boulder (USA)

Implementation and applications of the RASCI method with various spin-flip excitations: radicals, excited states, avoided crossings, conical intersections and more
D. Casanova.

15th International Congress on Catalysis
Munich (Germany)

O_2 activation by Ag impurities and CO oxidation on nanoporous gold. A computational study (Poster / Oral)
L.V. Moskaleva, S. Röhe, V. Zielasek, T. Klüner, K.M. Neyman, M. Bäumer

CO induced reconstruction of PdZn surface alloys (Poster)
C. Weilach, S. M. Kozlov, H. Holzapfel, K. M. Neyman, G. Rupprechter

Towards realistic models of nanostructures in catalysis described from first principles (Poster / Oral)
K.M. Neyman

24th American Chemical Society National Meeting
Philadelphia (USA)

Bases and Features of the Potential Energy Surface and Reaction Path Models, their Extensions and Beyond
Josep Maria Bofill Villà, Wolfgang Quapp, Marc Caballero

Moving on Strongly Correlated Potential Surfaces: Are there Alternatives to CAS-SCF
Peter Pulay, Josep Maria Bofill Villà

26th International Carbohydrate Symposium
Madrid (Spain)

The molecular mechanism of enzymatic glycosyl transfer with retention of configuration: evidence for a short-lived oxocarbenium ion-like species
C. Rovira

28th International Symposium on Rarefied Gas Dynamics (RGD 28)
Zaragoza (Spain)

Dynamics of Alkali Ions-Neutral Molecules Reactions: Radio Frequency-Guided Beam Experimental Cross-Sections and Direct Quasiclassical Trajectory Studies
J. Aguilar, J. de Andrés, J.M. Lucas, M. Albertí, F. Huarte-Larrañaga, D. Bassi and A.Aguilar

Cross Section Measurements for Dissociative and Chrage-Transfer Collisions Between Sodium Ions and $ZnBr_2$ Molecules
J. de Andrés, J.M. Lucas, M. Albertí, J.M. Bofill, A.Aguilar

Dynamics of Alkali Ions-Neutral Molecules Reactions: Radio Frequency-Guided Beam Experimental Cross-Sections and direct Quasiclassical Trajectory Studies.
J. Aguilar, J. de Andrés, JM. Lucas, M. Albertí, F. Huarte-Larrañaga, D. Bassi ,A. Aguilar.

Aalto Complex Networks Workshop
Sannäs Manor, Porvoo (Finland)

Networks meet Geometry: the S1 model
M.A. Serrano, D. Krioukov, M. Bogunyà

Advances in Quantum Chemistry: Interfacing electronic structure with dynamics
University of Minnesota, Minneapolis (USA)

How does nature break and form glycosidic bonds: QM/MM metadynamics investigations
C. Rovira

CECAM-Workshop: Enhancing Organocatalysis by Joining Advanced Theoretical and Experimental Approaches
Lugano (Switzerland)

Unravelling the Reaction Mechanism of Proline-Catalyzed Asymmetric Aldol Reactions in Water (Invited talk)
J.Ribas

CECAM-Workshop: Theoretical Challenges in Electronic Structure of Clusters and Nanoparticles
Lausanne (Switzerland)

Nanoclusters: real and hypothetical building blocks (Invited)
S. T. Bromley

CECAM-Workshop: "Modelling realistic inorganic nanostructures: Bridging the gap between theory and experiment"
Zaragoza (Spain)

Density functional studies of ceria nanostructures relevant for catalysis and beyond (Invited lecture)
K.M. Neyman, S.M. Kozlov

Realistic first principles description of Pd nanoparticles applied in catalysis and energy technologies (Invited lecture)
H.A. Aleksandrov, S.M. Kozlov, K.M. Neyman

CH_xO and CH_x species (x = 1-3) on a palladium nanoparticle representing model catalysts (Poster)
S.M. Kozlov, G.F. Cabeza, K.M. Neyman

Electronic structure and absolute energies of steps on CeO_2(111) (Poster)
S.M. Kozlov, F. Viñes, K. M. Neyman

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

COST Redox General Meeting 2012,
Prague (Czech Republic)

Exploring the electronic structure and optical excitations of F-doped TiO2: Relevance to Photocatalysis (Invited Lecture)
F. Illas

Crystal Forms at Bologna: 6th Bologna Convention on Crystal Forms
Bologna (Italy)

Theoretical studies of the properties of bistable molecular crytals using first-principles methods. (Invited talk)
J.J. Novoa

Departamento de Física de la Materia Condensada Universidad de Zaragoza

Zaragoza (Spain)

Modelización Computacional de Sistemas Magnéticos Moleculares
E. Ruiz

Dust in core-collapse supernovae near and far: understanding its formation and evolution
Monte Verità, Ascona (Switzerland)

A Bottom-up Approach to Dust Structure, Properties and Nucleation: Nano-silicates (Invited)
S. T. Bromley

Energy from the Sun: Computational Chemists and Physicists Take up the Challenge
Cagliary (Italy)

A computational investigation of organic dye-sensitized solar cells: the cyclopentadithiophene linker (Poster)
C. Climent, D. Casanova.

The conjugated linker's role in D-pi-A organic dyes: a computational study (Poster)

D. Casanova, C. Climent.

Equifases
Concepción **(**Chile)

Interpretation of multisite binding to macromolecules and functionalized particles in terms of the microscopic equilibrium constants
J.L. Garcés, C. David, C.; S. Madurga, I. Pastor, F. Mas, J. Puy, C. Rey-Castro

Esmolna
Cuenca (Spain)

Mononuclear Transition Metal Complexes: A Simple Alternative
E. Ruiz.

European Conference on the Dynamics of Molecular Systems (MOLEC 2012)
Oxford (United Kingdom)

Theoretical study of the dynamics and kinetics of the O + CS → CO + S chemical laser reaction, where CO shows a very high vibrational excitation
P. Gamallo, R. Francia, R. Martínez, R. Sayós, M. González

The dynamics of the $O(^3P)$ + CH_4 → OH + CH_3 reaction is similar to that of a triatomic reaction
R. Martínez, P.A. Enríquez, M.P. Puyuelo, M. González

Anatomy of the OH + D_2 → HOD(v_1',v_2',v_3') + D benchmark reaction from molecular beams and QCT-GB calculations
J.D. Sierra, D.R. Albert, H.F. Davis, L. Bonnet, M. González

Detailed resonance analysis in the Ne + H_2^+(v_0=2, j_0=1) → NeH^+(v'=0, j') + H proton transfer reaction. A challenge for experiment
P. Gamallo, F. Huarte-Larrañaga, M. González

Theoretical study of the dynamics and kinetics of the O + CS → CO + S chemical laser reaction, where CO shows a very high vibrational excitation
P. Gamallo, R. Francia, R. Martínez, R. Sayós, M. González

Detailed resonance analysis in the Ne + H_2^+(v_0=2,j_0=1) → NeH^+(v'=0,j') + H proton transfer reaction. A challenge for experiment.
P. Gamallo, F. Huarte-Larrañaga, M. González

First International Training School on NanoAlloys (ISNA)
Tirrenia, Pisa (Italy)

Realistic models of palladium nanoparticles for hydrogen storage (Poster)
H.A. Aleksandrov, S.M. Kozlov, K.M. Neyman

Arrangement of components in PdZn surface nanoalloy films on Pd(111) modified by CO adsorption (Poster)
C. Weilach, S.M. Kozlov, H. Holzapfel, K. Föttinger, K.M. Neyman, G. Rupprechter

First Ph. D. Workshop of the European Doctorate in Theoretical Chemistry and Computational Modeling
Barcelona (Spain)

Nanoeffects on properties of model catalytic systems: Intermetallic PdZn films on Pd(111) (Oral)
S.M. Kozlov

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

FunMol CECAM

Bonn (Germany)

Mononuclear Transition Metal Complexes: A Simple Alternative
E. Ruiz

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

Recent progress in density functional studies of ceria-based nanostructures (Oral)
K.M. Neyman

Adsorption induced rearrangement of PdZn surface alloys (Poster)
H.H. Holzapfel, C. Weilach, S.M. Kozlov, K.M. Neyman, G. Rupprechter

HPC-Europa2 Transnational Access Meeting (TAM)
Amsterdam (The Netherlands)

Modification of palladium nanoparticles by the surface and subsurface H and C species (Oral)
H.A. Aleksandrov, K.M. Neyman

The effect of mono- and multivalent ions on the electrostatic properties of a charged spherical colloid. Molecular dynamics study (Oral)
M. Nedyalkova, S. Madurga

ICIQ
Tarragona (Spain)

Single Ion Magntes based on 3d Metal Atoms: Analysis and New Candidates
E. Ruiz

ICMM-2012 (13th International Conference on Molecule-based Magnets)
Orlando (USA)

Bistability in the TTTA molecule-basd magnet. (Contributed talk)

J.J. Novoa

Innovación docente en Química (INDOQUIM 2012)
Barcelona (Spain)

Programas educativos de equilibrio de fases bajo la plataforma del Campus Virtual. Sistemas de un componente
S. Madurga, F. Mas, J. Ignés

In Silico Enzyme Design and Screening
International Centre for Theoretical Physics, Trieste (Italy)

Molecular dynamics based studies on human DPP III revealed determinants for its broad substrate selectivity
S. Tomić, A. Tomić, M. González

International Conference on Mathematical Methods in Science and Engineering (CMMSE 2012): Minisymposium on "From clusters to the solid state"
La Manga, Murcia (Spain)

Prediction of Stable Low Density Materials Inspired by Nanocluster Building Block Assembly (Invited)
S. T. Bromley

International Congress of the Spanish Biophysical Society (SBE-12)
Barcelona (Spain)

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

Fractal trajectory of a diffusing particle in 2D crowded media investigated by Monte Carlo simulations
L. Pitulice, E. Vilaseca, A. Isvoran, S. Madurga, I. Pastor, J.L. Garcés, F. Mas, F

Diffusion of particles with physiological molecular weights within extracellular gels used in 3D cultures
R. Galgoczy, I. Pastor, A. Colom, A. Giménez, F. Mas, J. Alcaraz

International School of Quantum Electronics: 53rd Course Molecular Physics and Plasmas in Hypersonics II
Erice (Italy)

Molecular reaction dynamics at surfaces
R. Sayós

International workshop "Understanding Chemical Reactivity: from modeling to experiment"
Bilbao (Spain)

Understanding dehydrohalogenations reactions induced by alkali ions: Experimental and Theoretical reaction dynamics studies

J. Aguilar, J.M. Lucas, F. Huarte-Larrañaga, M. Albertí, J. de Andrés and A. Aguilar

IX International Conference on "Mechanisms of Catalytic Reactions" (MCR-2012)
St. Petersburg (Russia)

Catalysis from first principles: Is it crucial to account for the effects of nanostructuring? (Keynote lecture)
K.M. Neyman

Joint Working Group Meetings of the COST-MP0903 Action "Nanoalloys as Advanced Materials: From Structure to Properties and Applications"
Antalya (Turkey)

Comparison between Pd-based intermetallic compounds and bimetallic alloys using density functional methods (poster)
S.M. Kozlov, K.M. Neyman

Materials Chemistry Consortium Meeting 2012
University College London, London (United Kingdomt)

Combinatorial Complexity in Nanosystems (Invited)
S. T. Bromley

Master Química V
Barcelona (Spain)

Estudi Montecarlo de la difusió 2D en medis densos
S. Alonso, I. Pastor, S. Madurga, F. Mas, E. Vilaseca

Mesilla Chemistry Workshop Ligand-Based Control of Spin and Reactivity in Metal Complexes
Mesilla (Mexico)

Spin-state Controlled Trigonal Twist of Six-Coordinate Transition Metals
S. Alvarez.

National Institutes of Health Seminars
Washington DC (USA)

Multireference systems with a single reference method: avoided crossings, conical intersections, multiradical character and more.
D. Casanova.

NoSIC-5 (Not Strictly Inorganic Chemistry)
Prullans de Cerdanya (Spain)

Chemistry and Poetry in Raymond Queneau's Cosmography
S. Alvarez.

Quantum Chemistry in the Solid State: Magnetic Coupling and Excited States on the Ocassion of the 60th Birthday of Prof. Ria Broer
Groningen (The Netherland)

The light-induced spin-crossover process in the $[Fe(bpy)_3]^{2+}$ complex (Invited Lecture)
C. Sousa

Quantum Days in Bilbao 2012: "Understanding Chemical Reactivity: from modeling to experiment"
University of Basque Country, Bilbao (Spain)

A quantum MCTDH study of H_2 confined in a SWCNT.
J. Suárez, F. Huarte-Larrañaga

Understanding dehydrohalogenations reactions induced by alkali ions: Experimental and Theoretical reaction dynamics studies
J. Aguilar, J.M. Lucas, F. Huarte-Larrañaga, M. Albertí, J. de Andrés and A. Aguilar

RGD28: 28th International Symposium on Rarefied Gas Dynamics
Zaragoza (Spain)

Molecular dynamics study of hydrogen atomic recombination over silica based on a new analytical DFT potential energy surface
P. Gamallo, M. Rutigliano , S. Orlandini , M. Cacciatore, R.Sayós

Satellite Workshop "In situ spectroscopy and model catalysis" of the 15th International Congress on Catalysis
Kloster Andechs / Munich (Germany)

First-principles modelling of nanostructures in catalysis and energy technologies (invited lecture)
K.M. Neyman

SPIE OPTO Oxide-based Materials and Devices III
Moscone Center, San Francisco (USA)

Structure and properties of nano-oxides: a theoretical overview (Invited)
S. T. Bromley

University of Assiut
(Egypt)

Theoretical Approach to Molecular Magnetism
E. Ruiz

University of Sohag
(Egypt)

Theoretical Approach to Molecular Magnetism
E. Ruiz.

VI European Workshop on Molecular Magnetism (JUJOLS VI)
Sevilla (Spain)

Bistability in molecule-based magnets. The TTTA case. (Invited talk)
J.J. Novoa

Photocycle of the light-induced spin-crossover process in the $[Fe(bpy)_3]^{2+}$ complex (Contributed Lecture)
C. Sousa

VII Trobada de Joves Investigadors dels Països Catalans
Palma de Mallorca (Spain)

Estudi computacional de colorants orgànics per la millora de l'eficiència de cel·les solars de Grätzel: el pont ciclopentaditiofè (CPDT)
C. Climent

Ab-initio I dinàmica directa en la reacció i-C_3H_7Cl + Na^+
J. Aguilar, E. López, J.M. Lucas, F. Huarte-Larrañaga, M. Albertí, J. De Andrés and A. Aguilar

Dinàmica de la reacció entre i-C_3H_7Br i Li^+
E. López, J. Aguilar, j. De Andrés, J.M. Lucas, M. Albertí and A. Aguilar

Natura de la correlació electrònica en DFT: de les molècules senzilles als complexos de titani
Marc Caballero, Iberio de P.R. Moreira, Josep Maria Bofill

Winter Modeling: Special Edition, A workshop to celebrate Prof. Vincenzo Barone on the Ocassion of his 60th Birthday
Pisa (Italy)

A quantum leap on surface modeling: from atoms on graphite to Pt nanoparticles on ceria (Invited Lecture)
F. Illas

Workshop on 'Nano-biocolloidal materials and non-equilibrium self-assembly'
Barcelona (Spain)

Diffusion in macromolecular crowded media: Monte Carlo simulation of obstructed diffusion vs. FRAP experiments
I. Pastor, E. Vilaseca, L. Pitulice, S. Madurga, J.L. Garcés, A. Isvoran, M. Cascante, F. Mas

Workshop on High-Dimensional Quantum Dynamics.
University of Birmingham, Birmingham (United Kingdom)

H_2 confined in CNTs: A Full Quantum 5-D study.

J. Suárez, F. Huarte-Larrañaga

World Resources Forum 2012
National Conference Center, Beijing (China)

Nanoscale Ceria: What Can Computational Modelling Tell Us? (Keynote)
S. T. Bromley

X Girona Seminar on Theoretical and Computational Chemistry for the Modeling of Biochemical Systems: From Theory to Application
Universitat de Girona, Girona (Spain)

How does nature break and form glycosidic bonds
C. Rovira

XIII Escuela Nacional de Materiales Moleculares
Peñíscola (Spain)

Theoretical studies of the properties of bistable molecular crystals using first-principles methods. (Invited talk)
J.J. Novoa

XVIII Congreso de Física Estadística, FisEs'12
Palma de Mallorca (Spain)

Networks meet Geometry: the S1 model and beyond
M.A. Serrano, M. Bogunyà

XV International Symposium on Luminiscence Spectrometry (ISLS2012)
Barcelona (Spain)

Diffusion of alpha-chymotrypsin in solution crowded media. A Fluorescence Recovery after Photobleaching study
I. Pastor, E. Vilaseca, S. Madurga, J.L. Garcés, M. Cascante, F. Mas

XXIII Sitges Conference: Understanding and Managing Randomnes in Physics, Chemistry and Biology
Sitges (Spain)

Diffusion in macromolecular crowded media: Monte Carlo simulation of obstructed diffusion vs. FRAP experiments
I. Pastor, E. Vilaseca, A. Isvoran, S. Madurga, J.L. Garcés, M. Cascante, F. Mas, F

XXVIII Reunió Anual de la Xarxa de Referència R+D+i en Química Teòrica i Computacional
Barcelona (Spain)

The key role of thermal fluctuations on the magnetic properties of the TTTA crystal. (Contributed talk)
S. Vela

Electronic structure and stability of steps on CeO_2(111) (Oral)
S.M. Kozlov, F. Viñes, K.M. Neyman

Estudi Montecarlo de la difusió 2D en medis densos
S. Alonso, I. Pastor, S. Madurga, F. Mas, E. Vilaseca

Estudi computacional de les propietats fotofísiques de complexos d'Ir(III)
C. Climent, D. Casanova , P. Alemany , P. Alam, I. R. Laskar

Experimental and theoretical dynamics study of the i-C_3H_7Cl +Li, Na, K ions reactions
J. Aguilar, J.M. Lucas, J. de Andrés, F. Huarte-Larrañaga, M. Albertí, A. Aguilar

Hydrogen confined in SWCNTs: Anisotropy effects on rovibrational quantum levels.
J. Suárez, F. Huarte-Larrañaga

Bandgap Engineering on Graphene (Invited talk)
F. Viñes

XXXII Reunión del Grupo de Electroquímico de la Real Sociedad Española de Química
Miraflores de la Sierra (Spain)

Películas delgadas de CuO dopadas con iones alcalinos mediante anodización de Cu. Estudio experimental y teórico de sus propiedades optoelectrónicas
F. Caballero-Briones, A. Palacios-Padrós, O. Calzadilla, I. de P. R. Moreira, F. Sanz *(Poster)*

XXXVIII Congresso de Químicos Teóricos de Expresion Latina
Natal (Brazil)

Towards the ab initio modeling of complex systems: Pt nanoparticles supported on ceria (Invited Lecture)
F. Illas

VISITING UNIVERSITIES AND RESEARCH CENTERS ABROAD

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

Invited Visiting Professor, Department of Chemical Physics and Zernike Institute for Advanced Materials. Gener 2012.

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

Invited Visiting Professor, Departamento de Ciencias Químicas y Farmacéuticas. Març 2012.

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

Invited Visiting Professor, Dipartimento di Chimica. Març-Juny 2012.

A. Carreras **UCLA, Los Angeles (USA)**

Predoctoral training visit, Department of Chemistry and Biochemistry. Maig-Juliol 2012.

M. Llunell **Università degli Studi di Torino (Italy)**

Invited Visiting Professor, Dipartimento di Chimica. Juny 2012.

K.M. Neyman **Universität Erlangen-Nürnberg, Erlangen (Alemanya)**

Invited Visiting Alexander von Humboldt Scientist, Department of Chemistry and Pharmacy. Juliol-Agost 2012.

G. Aullón **Universidad de Concepción (Chile)**

Invited Visiting Professor, Centro de Biotecnología. Curs de 20 hores “Teoría del Funcional de la Densidad Aplicada al Estudio de la Estructura Electrónica, la Reactividad y la Caracterización de Compuestos Químicos”. Agost 2012.

PARTICIPATION IN COMPETITIVE FUNDED RESEARCH PROJECTS

Theoretical study of tunable photomagnetic compounds
Ria Broer, Universitat de Groningen and Universitat de Barcelona
08PR2650, 2009-2013
Nederlandse organisatie voor toegepast natuurweten-schappelijk onderzoek TNO (The Netherlands)

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

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 i Riera, Universitat de Barcelona
2009SGR-1041, 2009-2013
Agència de Gestió d'Ajuts Universitaris i de Recerca, Generalitat de Catalunya

Self-Organized Complexity and Self-Assembling Materials
Francesc Sagués, Universitat de Barcelona
2009SGR-1055, 2009-2013
Agència de Gestió d'Ajuts Universitaris i de Recerca, Generalitat de Catalunya

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

Ajuts de suport als grups de recerca de Catalunya
Marta Cascante Serratosa, Universitat de Barcelona
2009SGR-1308, 2009-2013
Agència de Gestió d'Ajuts Universitaris i de Recerca, Generalitat de Catalunya

Grup d'Estructura Electrònica
Santiago Alvarez Reverte, Universitat de Barcelona
2009SGR-1459, 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

Planetary entry integrated models (Phys4Entry)
Ramón Sayós Ortega, Universitat de Barcelona i Mario Capitelli, Universitat Bari (Italy)
242311, 2010-2014
7è Programa Marc, collaborative project, space exploration (Unió Europea)

Xarxa de Referència d'R+D+I en Química Teòrica i Computacional (XRQTC)
Francesc Illas i Riera, Universitat de Barcelona
306261, 2011-2012
Departament d'Innovació, Universitats i Empresa. Generalitat de Catalunya

Modelling Electronic Processes in Nano Semioonductors: Clusters, Wires and Tubes
Stefan T. Bromley, Universitat de Barcelona
A e-GAP2 Project, 2010-2012

Cellular structure, networks and motifs
Ramon Reigada Sanz, Universitat de Barcelona
BFU2010-21847-C02-02, 2011-2013
Dirección General de Investigación y Gestión del Plan nacional de I+D+I (MICINN)

New NMR methods and new concepts for studying biomolecules with dynamic interactions involved in signalin.
Miquel Pons Vallés, Universitat de Barcelona
BIO2010-15683, 2011-2013
Ministerio de Ciencia e Innovación (MCI)

The Chemical Cosmos: Understanding Chemistry in Astronomic Environments
Stefan T. Bromley, Universitat de Barcelona
CM0805, 2010-2013
European Framework for Cooperation in Science and Technology (COST)

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

Reducible oxide chemistry, structure and functions
Francesc Illas i Riera, (Spanish Representative in the Management Committee), Konstantin Neyman (Substitute Spanish Representative in the Management Committee), Universitat de Barcelona
CM1104, 2012-2016
European Framework for Cooperation in Science and Technology (COST)

Physicochemistry of ligand-polyelectrolyte iteractions of environmental and physiological interest
Francesc Mas Pujadas, Universitat de Barcelona
CTM2009-14612-C02-02, 2009-2012
Dirección General de Investigación y Gestión del Plan nacional de I+D+I (MICINN)

Kinetic and dynamics models and simulations of reactions in dissociated gas environments over ceramics of interest for aerospace industry
Ramón Sayós Ortega, Universitat de Barcelona
CTQ2009-07647, 2010-2013
Dirección General de Investigación y Gestión del Plan nacional de I+D+I (MICINN)

Quantum Reaction Dynamics of Polyatomic Systems and Modeling of gas physisorption in nanostructures: processes with energetic and environmental interest.
Fermin Huarte Larrañaga, Universitat de Barcelona
CTQ2009-12215/BQU, 2010-2013
Dirección General de Investigación y Gestión del Plan nacional de I+D+I (MICINN)

Chemical processes dynamics by molecular beams and theoretical methods
Antonio Aguilar Navarro, Universitat de Barcelona
CTQ2010-16709/BQU, 2011-2013
Dirección General de Investigación y Gestión del Plan nacional de I+D+I (MICINN)

Structure and Dynamics of Chemical Reactions by Extended Reaction Path Models and Wavefunction Theory.
Josep Maria Bofill Villà, Universitat de Barcelona
CTQ2011-22505, 2012-2014
Dirección General de Investigación y Gestión del Plan nacional de I+D+I (MICINN)

Electronic Structure and Properties of Inorganic Molecules and Solids
Eliseo Ruiz Sabin, Universitat de Barcelona
CTQ2011-23862-C02, 2012-2014

Dirección General de Investigación y Gestión del Plan nacional de I+D+I (MICINN)

Electronic Structure and Properties of Inorganic Molecules and Solids
Pere Alemany i Cahner, Universitat de Barcelona
CTQ2011-23862-C02-02, 2012-2014
Dirección General de Investigación y Gestión del Plan nacional de I+D+I (MICINN)

Theoretical study of oxidation reactions initiated by HO, O_3 y NO_3
Josep Maria Anglada Rull, CSIC
CTQ2011-27812, 2012-2014
Dirección General de Investigación y Gestión del Plan nacional de I+D+I (MICINN)

Theoretical study of the dynamics and kinetics of chemical reactions. Atmospheric chemistry, combustion processes, and applications to enzyme systems
Miguel González Pérez, Universitat de Barcelona
CTQ2011-27857-C02-01, 2012-2014
Dirección General de Investigación y Gestión del *Plan nacional de I+D+I (MICINN)*

Computer-aided Design and Synthesis of New Enzymatic Inhibitors with Potential Anticancer Activity
Jaime Rubio Martínez, Universitat de Barcelona
CTQ2011-29285-C02-02, 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, Universitat de Barcelona
CTQ2011-25871, 2012-2014
Dirección General de Investigación y Gestión del Plan nacional de I+D+I (MICINN)

Ab initio modelling of technologically relevant oxide, metallic and combined oxide/metallic materials: from nanoscale to bulk.
Francesc Illas i Riera, Universitat de Barcelona
FIS2008-02238, 2009-2013
Dirección General de Investigación y Gestión del Plan nacional de I+D+I (MICINN)

Design of Thin-Film Nanocatalysts for On-Chip Fuel Cell Technology (chipCAT)
Konstantin M. Neyman, Universitat de Barcelona
FP7-NMP-2012-SMALL-6-310191, 2012-2016
European Comission Framwork Programme 7

Consulting on Photocatalysis
Francesc Illas i Riera
INAEL, 2011-2012

Magnetic properties and phase transitions in crystals with technological interest
Juan J. Novoa Vide, Universitat de Barcelona
MAT2011-25972.2012, 2012-2014
Ministerio de Economia y Competitividad

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

Metabolic Flux Analysis and Cancer (METAFLUX)
Marta Cascante Serratosa, Universitat de Barcelona
PITN-GA-2010-264780, 2010-2014
Comissió Europea (FP7-People)

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 i Riera, Universitat de Barcelona
PRI-PIBIN-2011-1028, 2012-2014
Ministerio de Economia y Competitividad

Developing models for Density Functional studies of hydrogen storage in metals to account for the effect of nanostructuring
Konstantin Neyman, Universitat de Barcelona
SB2010-0172, 2011-2012
Ministerio de Educación (MEDU)

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'

Contracte programa del Institut de Química Teòrica i Computacional de la Universitat de Barcelona (IQTCUB)
Francesc Illas i Riera, Universitat de Barcelona
2012
Universitat de Barcelona

Divulgació de la Química Teòrica i Computacional a l'Ensenyament Secundari.
Josep Maria Bofill Villà, Universitat de Barcelona
2012

Secretaria d'Universitats i Recerca del Departament d'Economia i Coneixement, Generalitat de Catalunya


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