



UNIVERSITAT DE BARCELONA



CeRQT



Centre especial de Recerca en Química Teòrica

Activity Report 2001-2003

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Introduction

The *Centre Especial de Química Teòrica* was approved by the *Comissió de Política Científica* on the 24th of March 1999 and by the Junta de Govern on the 15th of April 1999. The *Centre Especial de Química Teòrica* was set up by Research groups belonging to different departments of the *Universitat de Barcelona* and carry out their research in the field of Theoretical Chemistry and applications which range from the study of elementary reactions, the study of biomolecules, magnetic materials either organic or inorganic to material science and heterogeneous catalysis.

The research activity of this centre will benefit the Research Community by:

- Increasing the scientific projection of the Universitat de Barcelona in a field as broad and relevant as Theoretical Chemistry.
- Gathering together researchers with different background, areas of knowledge and skills but sharing common goals. Presenting a global and coordinated image of the research in Theoretical Chemistry carried out in the Universitat de Barcelona in order to be competitive at the international level.
- Strengthening interdisciplinary work between the several research groups and bringing their activity to a common ground with experimental research groups working in the field of surfaces, colloids, macromolecules and new material design.
- Promoting discussion on actual issues in Chemistry, either academical or fundamental and applied science.
- Sharing and efficiently managing the resources available at the different research groups.

One of the internal goals is strengthening the constitution of a third cycle of excellence and promoting high level scientific formation activities, as well as optimizing PhD programs and other educational activities of the and other educational activities of the *Universitat de Barcelona*. This will be achieved by globalizing the different individual activities of the groups toward the formation of researchers in Theoretical Chemistry. In this sense the work done in the last three years by the groups constituting the CeRQT has to be pointed out. At an academic level the centre has been involved in the “*Química Teòrica y Computacional*” inter-university PhD program. This program has been given the “*Mención de Calidad*” prize by the “*Ministerio de Educación, Ciencia y Cultura*” (Spanish Ministry for Education, Science, and Culture). At a scientific level the good results obtained by the funded research

project have to be highlighted, as well as the productivity measured in terms of work published in high impact publications or number of citations. The members of the centre have also actively participated in the organization of a large number of international conferences or meetings. The centre has also incorporated 8 researchers within the “*Ramón y Cajal*” program. Finally several member of the CeRQT have obtained prizes regarding their research: the “*Premio Solvay de Investigación Química*” Prize given by the CEOE Foundation to Dr. Santiago Olivella in 2002 and to Dr. Santiago Álvarez in 2003, the “*Premio de Investigación en Química Inorgánica*” awarded to Dr. Santiago Álvarez in 2003 by the “Real Sociedad Española de Química”, the distinction by the “Generalitat de Catalunya” in the promotion of University Research given to Dr. Santiago Álvarez in 2000 and to Dr. Francesc Illas in 2001 as senior researchers, and to Dr. Pere Alemany in 2002, Dr. Eliseo Ruíz, and Dr. Carme Rovira, both in 2003, as junior researchers. The information detailed in the following pages is a proof of not only of the potentiality of the CeRQT but also the success of this initiative.

CeRQT Directive Committee
January, 2004

CeRQT research areas and scientific production

The research projects of the CeRQT include both pure methodological projects as well as applications of theoretical methods to problems of current relevance in physics, chemistry and biology. The main research lines are the following:

- ✓ Theory and modeling of the kinetics and dynamics of chemical reactions: derivation of potential energy surfaces and treatment of the nuclear motion by means of quasiclassical. Semiclassical and quantum methods.
- ✓ Modeling of surfaces and solids. Reaction mechanisms in heterogeneous catalysis. Modeling of supported catalysts and electrochemical reactions. Magnetism in high Tc superconductors and other ionic solids.
- ✓ Molecular electronic structure and reactivity. Molecular stationary point optimization algorithms. Gas phase reactions. Reaction mechanisms relevant in atmospheric chemistry.
- ✓ Bonding, structure and properties of molecules and solids. Magnetic interactions in inorganic complexes. Structure and design of organic molecular crystals with magnetic, conducting or superconducting properties.
- ✓ Non-linear chemical reactions: front propagation, chaotic dynamics in space and time.
- ✓ Complex fluids: liquid crystals, polymeric and colloidal materials.
- ✓ Structure and properties of liquids and solutions. Solvent effect.
- ✓ Physicochemistry of macromolecules of environmental interest. Macromolecular complexation mechanisms. Biophysics of ligand-protein interactions.

Brief summary of the scientific production

Scientific production of the center during the period 2001-2003:

- ✓ 239 papers have been published in specialized scientific journals
 - ✓ More than 40 conferences have been given
 - ✓ 9 PhD thesis have been defended
 - ✓ 59 scientific projects have been financed by several national and international institutions.
- The total amount of the support reaches 4.400.000 €.

Publications classified by journals

Journal	N° of publications	Impact factor (2001)
Journal of Chemical Physics	34	2.998
Chemical Physics Letters	17	2.589
Chemistry - A European Journal	13	4.238
Physical Review B	12	3.327
Journal of Physical Chemistry A	12	2.765
Inorganic Chemistry	11	2.950
Journal of Physical Chemistry B	9	3.611
Physical Chemistry Chemical Physics	9	1.838
Journal of the American Chemical Society	8	6.201
Surface Science	8	2.140
European Journal of Inorganic Chemistry	4	2.526
International Journal of Quantum Chemistry	4	1.514
Journal of Computational Chemistry	4	2.931
Physical Review E	4	2.397
Theoretical Chemistry Accounts	4	1.421
Angewandte Chemie International Edition	3	7.671
Biochemical Journal	3	4.589
Chemical Communications	3	4.038
Dalton Transactions	3	3.023
Molecular Biology Reports	3	0.576
Organometallics	3	3.215
Polyhedron	3	1.414
Journal of Electroanalytical Chemistry	2	2.027
Chemical Physics	2	2.203
Chemistry of Materials	2	3.967
Contributions to Science	2	-
Crystal Engineering	2	-
European Journal of Biochemistry	2	2.999
International Journal of Molecular Science	2	-
Journal of Molecular Catalysis A	2	1.729
Journal of Solid State Chemistry	2	1.671
Journal of Theoretical Biology	2	1.552
Molecular Physics	2	1.617
Monatshefte fur Chemie	2	0.813
Organic Letters	2	3.715
Physical Review Letters	2	7.323
Journal of Physics: Condensed Matter	1	1.629
Applied Magnetic Resonance	1	0.673
Biochemical and Biophysical Research Communications.	1	1.494
Biochemical Society Transactions	1	2.205
Biochimica et Biophysica Acta	1	2.430
Biophysical Journal	1	4.636
Bioorganic and Medicinal Chemistry	1	2.051
Biotechnology ad Bioengineering	1	2.211

Catalysis Letters	1	1.559
ChemPhysChem	1	3.862
Drug Discovery Today	1	4.011
Electroanalysis	1	1.783
Environmental Science and Technology	1	3.123
European Journal of Nutrition	1	1.644
FEBS Letters	1	3.912
Haematologica	1	3.226
High Pressure Research	1	0.414
Inorganica Chimica Acta	1	1.566
International Journal of Modern Physics B	1	0.604
Journal of Agricultural and Food Chemistry	1	1.915
Journal of Biological Chemistry	1	6.696
Journal of Chromatography A	1	3.098
Journal of Inorganic Biochemistry	1	2.204
Journal of Magnetism and Magnetic Materials	1	1.046
Journal of Materials Chemistry	1	2.683
Journal of Molecular Catalysis B:Enzymatic	1	1.451
Journal of Molecular Structure THEOCHEM	1	1.014
Journal of Organic Chemistry	1	3.217
Journal of Organometallic Chemistry	1	1.901
Molecular Pharmacology	1	5.480
Nature Biotechnology	1	12.822
New England Journal of Medicine	1	31.736
New Journal of Chemistry	1	2.060
Pancreas	1	1.456
Physica B	1	0.609
Proceedings of the National Academy of Sciences of the USA	1	10.700
Radiation Effects and Defects in Solids	1	0.290
Structure and Bonding	1	5.194
Synthetic Metals	1	1.187
Toxicology	1	2.470

Organization and research groups of the CeRQT

The CeRQT is organized in a Directive Committee and a Center Committee. In the first stage of the Center (from its creation until October 11th, 2001) the Directive Committee was composed by:

Santiago Olivella, Director

Francesc Illas, Secretary

Santiago Alvarez, Vocal

From October 12th, 2001 on, the Directive Committee was composed by:

Francesc Illas, Director

Santiago Alvarez, Secretary

Antonio Aguilar, Vocal

The Center Committee is integrated by a representative from every CeRQT research group and among its tasks is choosing the Director Committee. Currently the Center Committee is composed by Drs. Francesc Illas, Santiago Alvarez, Antonio Aguilar, Eudald Vilaseca, Josep Maria Bofill, Marta Cascante and Francesc Sagués

Currently, the following research groups integrate the CeRQT:

- ✓ Research group on Integrative Biochemistry and Cancer Therapy (Department of Biochemistry and Biology)
- ✓ Research group on Kinetics and Dynamics of Elementary Reactions (Department of Physical Chemistry)
- ✓ Research group on Non-linear Dynamics (Department of Physical Chemistry)
- ✓ Research group on Physicochemistry of Macromolecular Systems or Colloids of Environmental Interest (Department of Physical Chemistry and Chemistry Department of the Lleida University)
- ✓ Research group on Electronic Structure (Departments of Physical Chemistry and Inorganic Chemistry)
- ✓ Research group on Quantum Chemistry of Materials (Physical Chemistry Department)
- ✓ Research group on Computational and Theoretical Chemistry (Organic Chemistry and Physical Chemistry Departments, and CSIC)

Members and collaborators of the CeRQT

The CeRQT is formed currently by 8 full professors, 14 associate professors, 27 graduate students, 14 doctors with a temporary contract (assistant professors, and contracts on behalf of the “Ramon y Cajal” and “ICREA” programs) and 2 post-doctoral fellows, as well as several collaborators, visiting professors and computer technical staff. Next, the members of the CeRQT between 2001 and 2003 are listed:

Integrative Biochemistry and Cancer

Therapy group

Marta Cascante Serratosa	Full Professor
Vitali Selivanov	Visiting Professor
Antonio Ramos Montoya	Doctoral Fellow (Generalitat de Catalunya)
Pedro Vizán Carralcázar	Doctoral Fellow (Generalitat de Catalunya)
Silvia Marin Martínez	Doctoral Fellow (Generalitat de Catalunya)

Non Linear Dynamics group

Francesc Sagues Mestre	Full Professor
Ramon Reigada Sanz	Ramon y Cajal fellow
Sergio Alonso Muñoz	Doctoral fellow (FPI)
Antonio Pons Rivero	Doctoral fellow (FPU)

Kinetics and dynamics of elementary reactions group

Antonio Aguilar Navarro	Full Professor
Miguel González Pérez	Full Professor
Margarita Albertí Wirsing	Associate Professor
Jaime de Andrés Llopis	Associate Professor
Josep M. Lucas Alcorta	Associate Professor
Xavi Giménez Font	Associate Professor
Ramón Sayós Ortega	Associate Professor
Fermín Huarte Larrañaga	Ramon y Cajal fellow
Irene Miquel Plana	Assistant Professor
Carolina Oliva García	Assistant Professor
Joan Sogas Solé	Assistant Professor
Carina Arasa Cid	Doctoral fellow (FPI)
Pablo Gamallo Belmonte	Doctoral fellow (UB)
Javier González Aguilar	Doctoral fellow (CeRQT)
Ma_Fernanda González Gutiérrez	Doctoral fellow (FPI)
Jordi Mayneris Perxachs	Doctoral fellow (FPU)
Alejandro Rodríguez García	Doctoral fellow (FPI)
Marta Sabidó Espín	Doctoral fellow (FPI)

Statistics and complex systems simulation group

Francesc Mas Pujadas	Full Professor
Eudald Vilaseca Font	Associate Professor
Josep Lluís Garcés González	Assistant Professor (LRU)
Sergio Madurga Díez	Scientific collaborator

Fernando Ortega Saine	Doctoral fellow (CeRQT)
<i>Electronic structure group</i>	
Santiago Alvarez Reverter	Full Professor
Juan José Novoa Vide	Full Professor
Michel Verdaguer	Visiting Professor (ICREA)
Pere Alemany Cahner	Associate Professor
Fernando Mota Valeri	Associate Professor
Eliseo Ruiz Sabín	Associate Professor
Gabriel Aullón López	Ramon y Cajal fellow
Mercé Deumal Solé	Ramon y Cajal fellow
Carme Rovira Virgili	Ramon y Cajal fellow
Cédric Desplanches	Post-doctoral fellow (Marie Curie)
Miquel Llunell Marí	Assistant Professor
Antonio Rodríguez-Fortea	Assistant Professor
M. Angels Carvajal Barba	Doctoral fellow (CeRQT)
David Casanova Casas	Graduate student
Thomas Cauchy	Doctoral fellow (FPI)
Jordi Cirera Fernández	Doctoral fellow (FPU)
Iñigo García Yoldi	Scientific collaborator
Sébastien Le Roux	TMR post-doctoral fellow
Emiliana d'Oria	Doctoral fellow (FPI)
Ana A Palacios Ruíz	Doctoral fellow (FPI)
Jordi Ribas Ariño	Doctoral fellow (FPU)
<i>Quantum Chemistry of materials research group</i>	
Francesc Illas Riera	Full Professor
Maria Angels Garcia Bach	Associate Professor
Juan Carlos Paniagua Valle	Associate Professor
Carme Sousa Romero	Associate Professor
Konstantin Neyman	ICREA researcher
Stefan Bromley	Ramon y Cajal fellow
Nuria López Alonso	Ramon y Cajal fellow
Ibério de Pinho Ribeiro Moreira	Ramon y Cajal fellow
Annapaola Migani	Post-Doc Marie Curie
Javier Carrasco Rodríguez	Doctoral fellow (FPU)
David Domínguez Ariza	Doctoral Fellow (Generalitat de Catalunya)
Silvia González Pérez	Doctoral fellow (UB)
David Muñoz Ramo	Doctoral fellow (FPI)
Daniel Torres Rangel	Doctoral fellow (UB)
Francesc Viñes i Solana	Doctoral fellow (FI)
<i>Theoretical and Computational Chemistry group</i>	
Santiago Olivella Nello	Professor (CSIC)
Josep Maria Bofill Villà	Associate Professor
Albert Solé Sabaté	Associate Professor
Javier González Aguilar	Doctoral fellow (CeRQT)
Ma_ Fernanda González Gutiérrez	Doctoral fellow (FPI)
<i>Support staff</i>	
Edgar Ros	Computer technician

Publications by members of the CeRQT during the period 2001-2003

Integrative Biochemistry and Cancer Therapy group

- 1) **“Occurrence of paradoxical or sustained control by an enzyme when over expressed: necessary conditions and experimental evidence with regard to hepatic glucokinase”**, P. de Atauri, L. Acerenza, B. N. Kholodenko, N. de la Iglesia, J. Guinovart, L. Agius, M. Cascante, *Biochem. J.*, 355, 787-793 (2001).
- 2) **“Effect of several anions on the activity of mitochondrial malate dehydrogenase from pig heart”**, A. Ruggia, J. L. Gelpí, M. Busquets, M. Cascante, A. Cortés, *J. Mol. Cat. B: Enz.* 11, 743-755 (2001).
- 3) **“Wheat Germ Extract Decreases Glucose Uptake and RNA Ribose Formation but Increases Fatty Acid Synthesis in MIA Pancreatic Adenocarcinoma Cells”**, L. G. Boros, K. Lapis, B. Szende, B. Tömösközi-Farkas, A. Balogh, J. Boren, S. Marin, M. Cascante, M. Hidvégi, *Páncreas*, 23, 141-143 (2001).
- 4) **“The effect of thiamine supplementation on tumour proliferation: A metabolic control analysis study”**, B. Comín-Anduix, J. Boren, S. Martinez, C. Moro, J. J. Centelles, R. Trebukhina, N. Petushok, W.-N. P. Lee, L. G. Boros, M. Cascante, *Eur. J. Biochem*, 268, 4177-4182 (2001).
- 5) **“Relationships between inhibition constants, inhibitor concentrations for 50%inhibition: new ways of analysing data”**, A. Cortés, M. Cascante, M. L. Cárdenas, A. Cornish-Bowden, *Biochem. J.*, 357, 263-268 (2001).
- 6) **“Gleevec (STI571) influences metabolic enzyme activities and glucose carbon flow toward nucleic acid and fatty acid synthesis in myeloid tumor cells”**, J. Boren, M. Cascante, S. Marín, B. Comín-Anduix, J. J. Centelles, S. Lim, S. Bassilian, S. Ahmed, W.-N. P. Lee, L. B. Boros, *J. Biol. Chem.*, 276, 37747-37753 (2001).
- 7) **“A new bis-indole, KARs. induces selective M arrest with specific spindle aberration in neuroblastoma cell line SH-SY5Y”**, B. Comín-Anduix, N. Agell, O. Bachs, J. Ovádi, M. Cascante, *Mol. Pharmacol*, 60, 1235-1242 (2001).
- 8) **“Product dependence and bifunctionality compromise the ultrasensitivity of signal transduction cascades”**, F. Ortega, L. Acerenza, H.V. Westerhoff, F. Mas, M. Cascante, *Proc. Nat. Acad. Sci. of the USA*, 99, 1170-1175 (2002).
- 9) **“Dependence of control coefficient distribution on the boundaries of a metabolic system: a generalized analysis of the effects of additional input and output reacionts to a linerar pathway”**, P. de Atauri, D.A. Fell, C. Chassagnole, D. Magret, J.P. Mazat, M. Cascante, *J. Theor. Biol.*, 215, 239-251 (2002).
- 10) **“Metabolic control analysis in drug discovery and disease”**, M. Cascante, L. G. Boros, B. Comín-Anduix, P. de Atauri, J.J. Centelles, P.W.-N. Lee, *Nat. Biotech.*, 20, 243-249 (2002).

- 11) **“Multiple glucose 6-phosphate pools or channelling of flux in diverse pathways?”**, L. Agius, J. J. Centelles, M. Cascante, *Biochem. Soc. Trans.*, 30, 38- 43 (2002).
- 12) **“Cysteinyl-flavan-3-ol conjugates from grape procyanidins. Antioxidant and antiproliferative properties”**, J. L. Torres, C. Lozano, L. Julià, F. J. Sánchez-Baeza, J. M. Anglada, J. J. Centelles, M. Cascante, *Bioorg. Med. Chem.*, 10, 2497-2509 (2002).
- 13) **“Triosephosphate isomerase deficiency: genetic, enzymatic and metabolic characterization of a new case from Spain”** A. Repiso, J. Boren, F. Ortega, A. Pujades, J.J. Centelles, J.J. Vives-Corrons, F. Climent, M. Cascante, J. Carreras, *Haematologica*, 87, ECR12 (2002).
- 14) **“Imanitib and Chronic-Phase Leukemias”**, L. G. Boros, W.-N. P. Lee, M. Cascante, M., *N. Engl. J. Med.*, 347, 67-68 (2002).
- 15) **“Dependence of control coefficient distribution on the boundaries of a metabolic system: a generalized analysis of the effects of additional input and output reactions to a linear pathway”**, P. de Atauri, D. A. Fell, C. Chassagnole, D. Magret, J. P. Mazat, M. Cascante, *J. Theor. Biol.*, 215, 239-251 (2002).
- 16) **“Metabolic control analysis aimed at the ribose synthesis pathways of tumor cells: a new strategy for antitumor drug development”**, J. Boren, A. Ramos-Montoya, P. de Atauri, B. Comin-Anduix, A. Cortes, J. J. Centelles, W. M. Fredericks, C. J. F. Van Noorden, M. Cascante, *Mol. Biol. Rep.*, 29, 7-12 (2002).
- 17) **“Valorization of grape (*Vitis vinifera*) byproducts. Antioxidant and biological properties of polyphenolic fractions differing in procyanidin composition and flavonol content”**, J. L. Torres, B. Varela, M. T. García, J. Carilla, C. Matito, J. J. Centelles, M. Cascante, X. Sort, R. Bobet, *J. Agr. Food. Chem.*, 50, 7548-7555 (2002).
- 18) **“Fermented wheat germ extract inhibits glycolysis/pentoses cycle enzymes and induces apoptosis through poly(ADP-ribose) polymerase activation in Jurkat T cell leukemia tumor cells”**, B. Comin-Anduix, L. G. Boros, S. Marin, J. Boren, C. Callol-Massot, J.J. Centelles, J.L. Torres, N. Agell, S. Bassilian, M. Cascante, *J. Biol. Chem.*, 277, 46408- 46414 (2002).
- 19) **“Cation-exchange micropreparative separation of galloylated and non-galloylated sulphur conjugates catechins”**, C. Lozano, M. Cascante, J. L. Torres, *J. Chromatog. A*, 973, 229-234 (2002).
- 20) **“Metabolic profiling of cell growth and death in cancer: Applications in drug discovery”**, L. G. Boros, M. Cascante, W.-N. P. Lee, *Drug. Discov. Today*, 7, 18-26 (2002).
- 21) **“Recent advances on the study of epigenetic effects induced by phycotoxin okadaic acid”**, E.E. Creppy, A. Traore, I. Baudrimont, M. Cascante, M.R. Carratu, *Toxicology*, 181-182, 433-439 (2002).
- 22) **“Modulation of metabolite concentrations with no net effect on fluxes”**, M. L. Cárdenas, F. Ortega, M. Cascante, A. Cornish-Bowden, *Mol. Biol. Rep.*, 29, 17-20 (2002).

- 23) **“Sensitivity analysis of metabolic cascades catalized by bifunctional enzymes”**, F. Ortega, M. Ehrenberg, L. Acerenza, H. V. Westerhoff, F. Mas, M. Cascante, *Mol. Biol.Rep.*, 29, 211-215 (2002).
- 24) **“Antiproliferative effect of antioxidant polyphenols from grape murine in Hepa-1c1c7”**, C. Matito, F. Mastorakou, J. J. Centelles, J.L. Torres, M. Cascante, *Eur. J. Nut.*, 42, 43-49 (2003).
- 25) **“Mathematical modelling of the urea cycle”**, A. Maher, P. Kuchel, F. Ortega, P. de Aauri, J. J. Centelles, M. Cascante, *Eur. J. Biochem.*, 270, 3953-3961 (2003).
- 26) **“Multicriteria optimisation of biochemical systems by linear programming: application to production of ethanol by *Saccharomyces cerevisiae*”**, J. Vera, P. de Aauri, M. Cascante, N.V. Torres, *Biotech. Bioeng.*, 83, 335-343 (2003).
- 27) **“The stable isotope-based dynamic metabolic profile (SIDMAP) of butyrate induced HT29 cell differentiation”**, J. Boren, W. N. P. Lee, S. Bassilian, J. J. Centelles, S. Lim, S. Ahmed, L. G. Boros, M. Cascante, *J. Biol. Chem.*, 278, 28395-28402 (2003).
- 28) **“Glucose conversion by multiple pathway in brain extract: theoretical and experimental analysis”**, F. Orosz, G. Wagner, F. Ortega, M. Cascante, J. Ovadi, *Biochemical and Biophysical Res. Comm.*, 309, 792-797 (2003).
- 29) **“Characterization of the transit and transition times for pathway unit of Michaelis-Menten mechanism”**, N. Sakamoto, P. de Aauri, M. Cascante, *Biochim. Biophys. Acta*, 1623, 6-12 (2003).
- 30) **“Defective RNA ribose synthesis in fibroblasts from patients with thiamin responsive megaloblastic anemia (TRMA)”**, L. G. Boros, M. P. Steinkamp, J. C. Fleming, W. N. Lee, M. Cascante, E. J. Neulfeld, *Blood*, *Epub ahead* (2003).
- 31) **“Metabolic strategy of boar spermatozoa revealed by a metabolomic characterization”**, S. Marín, K. Chiang, S. Bassilian, W.-N. P. Lee, L. G. Boros, J. M. Fernandez-Novell, J. J. Centelles, A. Medrano, J.E. Rodríguez-Gil, M. Cascante, *FEBS Letters*, 554, 342-346 (2003).

Five most cited publications of the group:

“Use of implicit methods from general sensitivity theory to develop a systematic-approach to metabolic control. 2. Complex systems”, M. Cascante, R. Franco, E. I. Canela, *Math. Biosci.*, 94, 289-309 (1989). 56 cites

“Use of implicit methods from general sensitivity theory to develop a systematic-approach to metabolic control. 1. Unbranched pathways”, M. Cascante, R. Franco, E. I. Canela, *Math. Biosci.*, 94, 271-288 (1989). 46 cites

“Oxythiamine and dehydropiandrosterone inhibit the nonoxidative synthesis of ribose ad tumor cell proliferation”, L. G. Boros, J. Puigjaner, M. Cascante, W. N. P. Lee, J. L. Brandes, S. Bassilian, F. I. Yusuf, R. D. Williams, P. Muscarella, W. S. Melvin, W. J. Schirmer, *Cancer Res.*, 57, 4242-4248 (1997). 34 cites

“The puzzle of the Krebs citric acid cycle: Assembling the pieces of chemically feasible reactions, and opportunism in the design of metabolic pathways during evolution”, E. MelendezHevia, T. G. Waddell, M. Cascante, *J. Mol. Evol.*, 43, 293-303 (1996). 24 cites

“Composite control of cell-function-metabolic pathways behaving as single control units”, B. N. Kholodenko, S. Schuster, J. M. Rohwer, M. Cascante, H. V. Westerhoff, *FEBS Lett.*, 368, 1-4 (1995). 19 cites

Non Linear Dynamics group

- 1) “**Noise-induced brownian motion of spiral waves**”, S. Alonso, F. Sagues, *Phys. Rev. E*, 63, 046205 (2001).
- 2) “**Regular wave propagation out of noise in chemical active media**”, S. Alonso, I. Sendiña-Nadal, V. Perez- Muñuzuri, J. M. Sancho, F. Sagues, *Phys. Rev. E*, 87, 078302 (2001).
- 3) “**Inertial effects on reactive particles advected by turbulence**”, R. Reigada, F. Sagues, J. M. Sancho, *Phys. Rev. E*, 64, 026307 (2001).
- 4) “**Turbulent advection of reacting substances**”, A. C. Martí, F. Sagués, *Physica A*, 295, 77 (2001).
- 5) “**Excitability transitions and wave dynamics under spatiotemporal structured noise**”, S. Alonso, F. Sagues, J. M. Sancho, *Phys. Rev. E*, 65, 066107 (2002).
- 6) “**Wave pattern dynamics in fluctuating media**”, F. Sagues, S. Alonso, J. M. Sancho, *Int. J. Mod. Phys. C* 13, 1243 (2002).
- 7) “**Quantitative analysis of Chemoconvection Patterns in the Methylene Blue-Glucose System**”, A. J. Pons, F. Sagues, M. A. Bees, P. G. Sorensen, *J. Phys. Chem. B* 106, 7252 (2002).
- 8) “**Traveling Waves and Nonequilibrium Stationary Patterns in Two-Component Reactive Lagmuir Monolayers**”, R. Reigada, F. Sagues, A. S. Mikhailov, *Phys. Rev. Lett.* 89, 038301 (2002).
- 9) “**Nonlinear chemical dynamics**”, F. Sagues, I. Epstein, *Dalton Trans.* 1201 (2003).

Five most cited publications of the group:

“**External fluctuations in front propagation**”, J. Armero, J. M. Sancho, J. Casademunt, A. M. Lacasta, L. Ramírez-Piscina, F. Sagues, *Phys. Rev. Lett.*, 76, 3045-3048 (1996). 25 cites

“**Wave propagation in a medium with disordered excitability**”, I. Sendina-Nadal, A. P. Munuzuri, D. Vives, V. Pérez-Munuzurri, J. Casademunt, L. Ramírez-Piscina, J. M. Sancho, F. Sagues, *Phys. Rev. Lett.*, 80, 5437-5440 (1998). 25 cites

“**Brownian motion of spiral waves driven by spatiotemporal structured noise**”, I. Sendiña-Nadal, S. Alonso, V. Perez-Muñuzurri, M. Gomez-Gesteira, V. Perez-Villar, L. Ramirez-Piscina, J. Casademunt, J. M. Sancho, F. Sagues, *Phys. Rev. Lett.*, 84, 2734-2737 (2000). 23 cites

“**Fluctuation-dominated kinetics under stirring**”, R. Reigada, F. Sagues, I. M. Sokolov, J. M. Sancho, A. Blumen, *Phys. Rev. Lett.*, 78, 741-744 (1997). 16 cites

“**Regular wave propagation out of noise in chemical active media**”, S. Alonso, I. Sendiña-Nadal, V. Perez-Muñuzurri, J. M. Sancho, F. Sagues, *Phys. Rev. Lett.*, 87, 078302 (2001). 11 cites

Kinetics and Dynamics of elementary reactions group

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Dr. Richard Hillary, “Langmuir circulations, lobe dynamics and plankton patch synchronisation”, 26th January, 2001

Dr. Davide Bassi, Dipartimento di Fisica. Università de Trento (Italy): “Bond forming ion-molecule reactions”, 14th February, 2001.

Dr. Paul Lee, Department of Pediatrics. Harbor-UCLA Research Center. California (U.S.A.): “Stable isotope methodology in review”, 19th February, 2001

Dr. Hans Westerhoff, Department of Microbial Biology, Vrije University, Amsterdam (Netherlands): “Control analysis in a changing world”, 1st March, 2001.

Dr. Juli Peretó, Universitat de Valencia: “Evolució prebiòtica: el camí cap a la vida”, 22th March, 2001.

Dr. Juli Peretó, Universitat de Valencia: “Evolució i metabolisme”, 23th March, 2001.

Dr. Phillip Kuchel, Department of Biochemistry, University of Sidney (Australia): “Using NMR to monitor metabolic processes in erythrocytes”, 26th March, 2001.

Dr. Pete Mulquiney, Department of Biochemistry, University of Oxford (U.K.): “Modelling the metabolism and function of the beating heart”, 26th March, 2001.

Dra. Wilma Frederiks, Department of Celbiologie and Histologie. Academisch Medisch Centrum. Universiteit van Amsterdam (Netherlands): “Enzyme histochemistry and oxidative stress in review”, 1st April, 2001.

Sra. Klazien Bosch, Department of Celbiologie and Histologie. Academisch Medisch Centrum. Universiteit van Amsterdam (Netherlands): “How to use enzyme histochemistry in tissues”, 2nd April, 2001.

Prof. Dr. Dario de Fazio, Università di Perugia, Perugia (Italy): “The $F + H_2 \rightarrow HF + H$ reaction: Open-shell, spin orbit and long-range effects”, 26nd April, 2001.

Dr. Xavier Giménez, Departament Química Física, Univ. Barcelona: “Aplicacions Moleculars de la Mecànica Semiclássica”, 29th May -1st June, 2001.

Dr. Giovanni di Gregorio, Dipartimento di Chimica Fisica, Università di Palermo (Italy). “**Estudio Monte Carlo del equilibrio conformacional de la N-hidroxiurea en agua**”, 2nd July, 2001

Prof. Dr. Carlo Petrongolo, Dipartimento di Chimica, Università di Siena, Italy: “Dynamics of the $N+H_2$ and $N+O_2$ reactive collisions. NO_2 spectroscopy”, 11th July, 2001.

Prof. Dr. Franco Vecchiocattivi, Università di perugia, Perugia (Italy): “Stereodynamic of collisional ionization processes”, 19th September, 2001.

Dr. Boris Kholodenko, Department Pathology, Anatomy and Cell Biology. Thomas Jefferson University. Philadelphia (U.S.A.): “Metabolic control of signal transduction”, 27th September, 2001.

Workshop on Transketolase and Glucose-6-phosphate deshydrogenase, the key enzymes in control of pentose phosphate metabolism. 9th November, 2001.

Prof. Dr. Joan Bertran, Universitat Autònoma de Barcelona, Conferències Magister del CeRQT. 1. “La clave de la catálisis enzimática”, 29th November 2001

Dra. Fabrizia Grepioni, Università di Sassari (Italy) “Organometallic polymorphism and phase transitions”, 14th December 2001

Dr. Miguel A. Rodríguez, Departamento de Química, Universidad de La Rioja: “Carbenos de Fischer: fotoquímica exploratoria de iminas de complejos metal-carbeno”, 20th December, 2001.

Prof. Dr. Ramon Carbó-Dorca, Universitat de Girona, Conferències Magister del CeRQT. 2. “Espais de Sovolev i funcions d’ona esteses”, 19th April 2002

Prof. Dr. Enrico Clementi, Università degli Studi della Insubria (Italy), Conferències Magister del CeRQT. 3. “Present status of the Hartree-Fock-Clementi-Corongiu method”, 17th May 2002

Dr. Manuel Almeida, Departamento de Química, Instituto Tecnológico y Nuclear, Sacavém (Portugal). “Transition metal bisdichalcogenates: useful building blocks for molecular materials and puzzling structural diversity”, 24th May 2002

Prof. Dr. J. R. Grijera, IFLYSIB (Instituto de Física de Líquidos y Sistemas Biológicos), Universidad Nacional de La Plata y CONICET, Argentina, “Termodinámica, dinámica y consecuencias de la interacción hidrofóbica”, 26th September 2002

Prof. Dr. Joel S. Miller, University of Utah (Salt Lake City, Utah, USA). “Extraordinary long (2.9 Å) C-C bonds: Supramolecular CC bonds?”, 4th October 2002

Prof. Dr. Paul Bagus, Texas A&M University (USA). Conferències Magister del CeRQT. 4. “Chemical information from core-level binding energy shifts: correct interpretations”, 8th November 2002.

Prof. Dr. Roald Hoffmann, Cornell University (USA). Conferències Magister del CeRQT. 5. “Electron-rich multicenter bonding in molecules and extended structures”, 20th December 2002

Prof. Dr. Armando Riera Compte, Departamento de Química, Facultad de Ciencias, Universidad Autónoma de Madrid. “Tratament teòric de col·lisions ió-àtom i ió-molècula”, 4th February 2003

Prof. Dr. Dario de Fazio, Dipartimento di Chimica, Università di Perugia CNR-IMIP (Italy). “Resonance effects in elementary chemical processes: the $F + H_2 \rightarrow HF + H$ reaction”, 4th April 2003

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Dr. Lluís Rovira, AGAUR. “Mapa de Excel·lència en Física i Química de les universitats espanyoles”, 30th May 2003

Dr. Florentino Borondo, Universidad Autonoma de Madrid. “¿Que es el caos? ¿Y el caos cuantico?”, 11th June 2003

Prof. Dr. E. Mizraji, Sección de Biofísica, Facultad de Ciencias, Universidad de la República, Montevideo (Urugay), “Modelización de sistemas neuronales”, 18th de June, 2003

Dr. Christoff Hartnig, Forschungszentrum Juelich, Germany. “Computer Simulations of Fuel Cell Membranes”, 3th July 2003

Prof. Dr. Eugene Kotomin, Max Planck Institute, Stuttgart, Germany, “A comparative theoretical study of perovskite surfaces”, 18th December 2003

Conferences organized by the CeRQT in the Barcelona Scientific Park (PCB) during 2001-2003

Dra. C. Rovira, “L'enllaç hemo-lligand a la mioglobina. Estructura i dinàmica”, 9th January, 2001.

Dr. C. de Graaf, “Acoplamiento magnético en compuestos de estado sólido: Interpretación y predicción teórica”, 6th February, 2001.

Dra. M. Cascante, “Eines teòriques per a l'estudi de xarxes de reaccions d'interés bioquímic”, 15th May, 2001.

Dr. E. Vilaseca, “Efecte del dissolvent. Estudi Monte Carlo de propietats moleculars en dissolució”, 25th June, 2001.

Dr. U. Manthe, Theoretische Chemie, TU Muenchen, Garching, Germany. “Quantum dynamics of polyatomic reaction processes”, 14th May 2002 (cancelled by Dr. Manthe due to health reasons)

Prof. Dr. P. Pulay, Department of Chemistry and Biochemistry, Fulbright College of Arts and Sciences, University of Arkansas, Fayetteville, Arkansas, USA. “Second order Møller-Plesset calculations for large molecules”, 5th July 2002

Prof. Dr. M. Parrinello, Swiss Center for Scientific Computing (CSCS), Manno, and Department of Chemistry, ETH, Hönggerberg HCI, Zurich, Switzerland, “Molecular dynamics: new approaches to the long time scale problem”, 6th September 2002

Prof. Dr. J. R. Grijera, IFLYSIB (Instituto de Física de Líquidos y Sistemas Biológicos), Universidad Nacional de La Plata y CONICET, Argentina, “Simulación por dinámica molecular: de gases a macromoléculas”, 27th September 2002

Dr. B. Moveghar, SOMS Centre, University of Leeds, Leeds, UK, **Prof. J. M. Ribó**, Departament Química Orgànica, Universitat de Barcelona, **V. Gomis**, Departament de Física Aplicada, Universitat Politècnica de Catalunya. “Electronic transport in low dimensional organic systems”, 15th January 2003

Prof. Dr. E. Mizraji, Sección de Biofísica, Facultad de Ciencias, Universidad de la República, Montevideo (Uruguay), “Modelos biofísicos para los procesos de memoria y razonamiento”, 27 de June, 2003

Internationals conferences and meetings (invitation and organization)during 2001-2003

Biochemistry and Cancer Therapy group

Dra. Marta Cascante

- * XIII Meeting of the European Association for red cell research, Barcelona, Spain 2001
- * Cellular signaling and metabolism: balancing between efficacy and damage, Moscú, Russia 2001
- * International Symposium on “Dietary Phytochemicals and Human Health, Salamanca, Spain 2002
- * Seminar EMBL (European Molecular Biology Laboratory). Metabolic networks - experimental and computational approaches, Heidelberg, Germany 2002
- * 10th International BioThermoKinetics Meeting (BTK 2002), Bordeaux, France 2002
- * Harbor-UCLA Symposium and Workshop on Metabolic Profiling and Metabolic Control Analysis, Los Angeles, USA 2002
- * NVBMB- Spring symposium on Systems , Biochemistry and disease, Amsterdam, Holanda 2003
- * Euromedlab Barcelona 2003. 15th IFCC-FESCC European Congress of Clinical Chemistry and Laboratory Medicine. 22nd National Congress of the Spanish Society of Clinical Biochemistry and Molecular Pathology, Barcelona, Spain 2003
- * 2^a European School of Computational Chemistry , Reaction and Molecular Dynamics: Lecture and tutorial on modelling metabolic pathways and identification of control steps, Barcelona, Spain 2003

Kinetics and dynamics of elementary reactions group

Dr. Antonio Aguilar

- * XIX International Symposium on Molecular Beams, Roma, Italy 2001
- * 5th Iberian Joint Meeting on Atomic and Molecular Physics , IBER2002, Lisboa, Portugal 2002
- * Final Evaluation Workshop of the COST D9 Action: Advanced Computational Chemistry of Increasingly Complex System, Smolenice, Eslovàquia, 2002.

Dr. Miguel González

- * Gordon Research Conference on Molecular Energy Transfer, Ventura, USA 2001

- * XVIIIth Internacional Conference on Molecular Energy Transfer (COMET XVIII), San Lorenzo de El Escorial, Spain 2003
- * VIIth Workshop on Quantum Reaction Dynamics, San Lorenzo de El Escorial, Spain 2003
- * 2nd European School on Computational Chemistry, Reaction and Molecular Dynamics”, Barcelona, Spain 2003

Non Linear Dynamics group

Dr. Francesc Sagués

- * Sixth SIAM Meeting on Applications of Dynamical Systems, Salt Lake City, USA 2001
- * School and Conference on Spatiotemporal chaos, Trieste, Italy 2002
- * Unsolved Problems of Noise, Washington, USA 2002
- * Trends in Pattern Formation: From Amplitude Equations to Applications, Dresden, Germany 2003
- * Dynamic Days, Palma de Mallorca, Spain 2003

Statistics and complex systems simulation group

Dr. Francesc Mas

- * **“Study of complex macromolecular binding systems. A hierarchical view of cooperativity”**, International Symposium Modelling Complex Biophysical Processes, Colonia de Sacramento, Uruguay 2002
- * **“Ion binding to natural organic matter: polyelectrolytic, heterogeneity and competitive effects”**, 2nd BIOSPEC (*Sensor development for routine prediction of metal bioptake in freshwaters and soil solutions*) meeting, Lleida, Espanya 2002

Fernando Ortega

- * **“Sensitivity analysis of metabolic cascades catalyzed by bifunctional enzymes”**, International BioThermoKinetics (BTK) meeting, Bordeaux-Arcachon, Francia 2002

Electronic Sctructure group

Dr. Santiago Álvarez

- * **“Comunicación visual en química”**, Curs Química, vida y comunicación: Imagen y realidad de la Ciencia del bienestar, Valladolid, Spain 2001
- * **“Cómo medir la simetría y la quiralidad a escala atómica”**, XXVIII Bienal de la Real Sociedad Española de Química. Madrid, Spain 2001
- * President del Comitè Organitzador, 6th FIGIPS Meeting in Inorganic Chemistry, Barcelona, 15-20 July 2001
- * **“Medidas Continuas de Simetría: Cómo (y por qué) medir la simetría y la quiralidad a escala atómica”**, IV Seminarios de Estudios Avanzados sobre Diseño Molecular y Bioinformática. Universidad de La Habana, Cuba 2002
- * **“Magnetismo Molecular: modelos teóricos y análisis computacional de las interacciones de intercambio”**, IV Seminarios de Estudios Avanzados sobre Diseño Molecular y Bioinformática. Universidad de La Habana, Cuba 2002
- * **“Symmetry, Chirality and Shape as Continuous Properties in Transition Metal Chemistry”**, 35th International Conference on Coordination Chemistry. Heidelberg, Germany 2002
- * President del Comitè Organitzador, NOSIC - Not Strictly Inorganic Chemistry, Prullans de Cerdanya, June 2003.
- * **“Polyhedra in Transition Metal Compounds: Symmetry, Shape and Chirality as Continuous Properties”**, 9th European Conference on Solid State Chemistry. Stuttgart, Germany 2003
- * **“Symmetry and Shape Measures in the Solid State”**, Gordon Research Conference Solid State Chemistry II. Oxford, UK 2003

Dr. Juan J Novoa

- * **“Low energy polymorphic forms of the acetic acid crystal. Ab initio DFT versus empirical atom-atom computations”**
CECAM Workshop “Computational methods for the simulation of organic and organometallic condensed phases”, Lyon, France 2001
- * **“Ab initio calculations on the crystal packing of acetic acid”**
20th European Crystallographic Meeting, Krakow, Poland 2001
- * **“On the existence of long C-C bonds between pairs of anions which repel: when and why? A test case on the [TCNE]₂²⁻ dimers found in ionic crystals”**,
CrystEngComm Discussion 1. Innovation in Crystal Engineering. Bristol, UK 2002

* **“Magnetism in Molecular Materials: From microscopic interactions to the macroscopic properties in a rigorous way”**,

CECAM Workshop “Electronic Structure Approaches to the Magnetic Behavior of Molecular-Based Materials: from the molecule to the Solid”, Lyon, France 2002

* **“Magnetism in Molecular Materials: What ab initio Calculations Tell us About its Microscopic and Macroscopic Properties”**,

International Congress on Molecular Based Magnets, Valencia, Spain 2002

* **“Theoretical study of the magnetism in molecular materials using ab initio quantum mechanical methods”**,

Meeting on Ab initio design of structural materials, Uppsala, Suecia 2003

* **“Unconventional OH...O bonds”**,

226th ACS National Meeting, New York, USA 2003

Dra. Carme Rovira

* **“Ab initio simulations of heme models”**, 2nd Car-Parrinello molecular dynamics workshop (CPMD 2001). Schloss Ringberg – München. Germany. 2001.

* **“Influence of the heme pocket on the structure and vibrations of the Fe-CO bond in myoglobin”**, CECAM workshop: Ab initio modeling in biology. Lyon. France. 2001.

* **“Binding of ligands to hemeproteins. A QM/MM investigation”**, CECAM workshop: Mixed or hybrid quantum/classical methods. Lyon. France. 2001.

* **“Modeling the ligand binding properties of myoglobin by first-principles molecular dynamics”**, Workshop on advances in first-principles computational condensed-matter physics. Tenerife. Spain. 2002.

* **“DFT investigation of the catalytic mechanism of catalases and peroxidases”**, Symposium on Nano-physics of life systems. Carlsberg Academy. Copenhagen. Denmark. 2002.

* **“The proximal hydrogen bonded residue controls the stability of the compound II intermediate in peroxidases and catalases”**, Second conference on quantum bioinorganic chemistry (QBIC-2). Örenas castle, Lünd. Sweden. 27-29. 2002.

* **“Ligand binding properties of hemeproteins modeled by first-principles molecular dynamics”**, EURESCO conference: Computational Biophysics: Integrating Theoretical Physics and Biology. San Feliu de Guixols, Spain. 2002.

Dr. Eliseo Ruíz

* **“Theoretical Study of the Exchange Coupling in Polynuclear Transition Metal Complexes”**, Molecular Magnets, European Science Foundation, Davos, Switzerland 2001

* **“Magnetic Materials with Transition Metals: Analysis and Design using Theoretical Tools”**, Materials Research Society Meeting, Boston, USA 2002

* **“Magnetic Materials with Transition Metals: Analysis and Design using Theoretical Tools”**, E-MRS Meeting, Strasbourg, France 2003

* **“Molecular Magnetism: Design and Understanding using Theoretical Tools”**, JOCS-03 (Jornades Catalanes de Supercomputació, Barcelona, Spain, October 2003

Grup de Química Quàntica de Materials

Dr. Francesc Illas

*Euroconference on **“Molecular Mechanisms of Heterogeneous Catalysis”** , San Feliu de Guíxols, Spain 2001

* **“Cluster Models in Computational Material Science”**, NATO ASI Computational Material Science, Il Ciocco, Italy 2001

* **“Ab initio study of magnetic interactions and determination of effective hamiltonian parameters in High Tc superconductors”**, Total Energy Methods in Computational Condensed Matter, Tenerife, Spain 2002

* **“Effective Hamiltonian parameters in High Tc superconductors from ab initio cluster model calculations”**, NATO Advanced Science Institute on Metal Ligand Interactions in Molecular, micro, macro and nano systems, Cetraro, Italy 2002

* **“Understanding charge-transfer processes at electrodes from a quantitative quantum-mechanical point of view”**, International Society of Electrochemistry, Dusseldorf, Germany 2002

* **“Structure and bonding of Pd clusters supported on α -Al₂O₃(0001)”**, International Workshop on the Structure and Reactivity of Oxide Surfaces, Sapporo, Japan, 2003

* **“NO reactivity on MgO surface defects: Low-coordinated ions, oxygen vacancies, and nickel impurities”**, 215 Meeting of the American Chemical Society, New Orleans, USA 2003

* **“The interaction of Pd atoms and clusters supported with a α -Al₂O₃(0001)”**, Euroconference on Nano-oxides: perspectives and applications of oxide based ultrathin films and nanoparticles, Brixen, Italy 2003

* **“Hacia una descripción mecano-cuántica *ab initio* de la transferencia electronica en electrodos”**, Centenario de la Real Sociedad Española de Química, Madrid, Spain 2003

* **“Transition metal atoms and clusters on oxide surfaces: structure and magnetic properties”**,The Applied Statistical Physics: Molecular Engineering Conference, Puerto Vallarta, Mexico 2003

Dr. Nuria Lopez

* **“First principles study on the properties of gold catalysts”**, 215 Meeting of the American Chemical Society, New Orleans, USA 2003. Title:.

Grup de Química Teòrica i Computacional

Dr. Josep Maria Bofill

* **“From Potential Energy Surface to Chemical Dynamics through Reaction Path Hamiltonian”**, 213 Meeting of the American Chemical Society, Florida, USA 2002

CeRQT Infrastructures and machinery.

Machinery currently available by the CeRQT:

- 2 clusters for massive computation. Each cluster has 15 Dell Optiplex nodes and 1 Dell Precision server, interconnected by a Gigabit Dell PowerConnect 5224 switch (cerqt.qt.ub.es-161.116.153.1 and hades.qt.ub.es-161.116.153.2).
- 1 cluster formed by 1 Dell Optiplex server and 3 multiprocessador Dell Precision nodes (alfa.qf.ub.es-161.116.83.20).
- 7 Dell Precision multiprocessor servers (davis.qi.ub.es-161.116.75.87, cannonball.qi.ub.es-161.116.75.88, trane.qi.ub.es-161.116.75.89, evans.qi.ub.es-161.116.75.90, carlit.qf.ub.es-161.116.73.30, taga.qf.ub.es-161.116.73.108 and cadi.qf.ub.es-161.116.73.165).
- 2 Dell PowerEdge 2600 multiprocessor servers.(count.qi.ub.es-161.116.75.122 and duke.qi.ub.es-161.116.75.113).
- 3 Compaq AlphaServer DS20E multiprocessor servers for intensive computation (ub222036.pcb.ub.es – 161.116.222.36, hal6006.qf.ub.es – 161.116.73.211 and cindy.qf.ub.es – 161.116.73.196).
- 3 HP J series multiprocessor servers (hal6004.qf.ub.es-161.116.73.175 (HPJ282), laser.qf.ub.es-161.116.73.196 (HPJ282) and hal6005.qf.ub.es-161.116.73.181 (HP J2240)).
- 5 Silicon Graphics Indygo2 multiprocessor servers (linus.qi.ub.es-161.116.75.18, turing.qi.ub.es-161.116.75.48, suanpan.qi.ub.es-161.116.75.50, keith.qi.ub.es-161.116.75.101 thelorious.qi.ub.es-161.116.75.102)
- 2 Dell Precision servers (atenea.qf.ub.es-161.116.73.232 and minerva.qf.ub.es-161.116.73.231).
- 40 PC workstations (pcb.ub.es (7), qf.ub.es (27), bq.ub.es (6)).
- 10 Mactintosh workstations (qf.ub.es).
- 1 HP Color LaserJet 4550 printer.
- 4 impressores HP LaserJet 2100/TN.
- 4 impressores HP LaserJet (1200 (3) and 1100 (1)).

Currently a cluster of 154 nodes is being negotiated.

Projects and funding of the CeRQT

Projects funded by the Spanish Government (CICYT)

TITLE OF THE PROJECT: Control de la proliferación tumoral mediante inhibidores de la síntesis de ribosa-fosfato: Efecto antagónico de la tiamina y sus derivados inactivos

PROGRAMME: Ayudas para proyectos de investigación del área de Ciencias de la Salud (FIS) (Proyecto 00/1120)

DURATION FROM: 2000 UNTIL : 2003

AMMOUNT FUNDED: 69.416,90 €

PROJECT LEADER: Dra. Marta Cascante Serratosa

TITLE OF THE PROJECT: Caracterización a nivel metabólico y celular de polifenoles bioactivos obtenidos a partir de subproductos de la industria agroalimentaria y forestal

PROGRAMME: Programa Nacional de Promoción General del Conocimiento (proyecto PPQ2000-0688-C05-04)

DURATION FROM: 2000 UNTIL : 2003

AMMOUNT FUNDED: 36.180,93 €

PROJECT LEADER: Dra. Marta Cascante Serratosa

TITLE OF THE PROJECT: Preparación de antioxidantes conjugados de cisteamina y flavanoles a escala semipiloto. Evaluación físico-química y toxicológica.

PROGRAMME: Ayudas a la Investigación (proyecto PTR1995-0611-OP)

DURATION FROM: 2002 UNTIL : 2004

AMMOUNT FUNDED: 83.660,00 €

PROJECT LEADER: Dr. Josep Ll. Torres

TITLE OF THE PROJECT: Obtención de procianidinas a partir de bagazo de uva y corteza de pino. Aplicaciones alimentarias y biomédicas.

PROGRAMME: Programa Nacional de Procesos y Productos Químicos (Proyecto PPQ2003-06602-C04-04)

DURATION FROM: 2003 UNTIL : 2006

AMMOUNT FUNDED: 65.000,00 €

PROJECT LEADER: Dra. Marta Cascante Serratosa

TITLE OF THE PROJECT: Una estrategia multidisciplinar en la búsqueda de nuevas dianas terapéuticas para el tratamiento del cáncer.

PROGRAMME: Programa Nacional de Promoción General del Conocimiento (proyecto SAF2002-02785)

DURATION FROM: 2002 UNTIL: 2005

AMMOUNT FUNDED: 121.300,00 €

PROJECT LEADER: Dra. Marta Cascante Serratosa

TITLE OF THE PROJECT: Dinámica no lineal en sistemas complejos: Autoorganización espacio-temporal y autoensamblaje en materia blanda.

PROGRAMME: Promoción General del Conocimiento (Proyecto BQU 2003-05042-C02-01)

DURATION FROM: 2003 UNTIL: 2006

AMMOUNT FUNDED: 134.000 €

PROJECT LEADER: Dr. Francesc Sagués

TITLE OF THE PROJECT: **Investigación teórica y práctica de procesos reactivos elementales entre iones y moléculas**

PROGRAMME: Promoción General del Conocimiento (Proyecto PB97-0919)

DURATION FROM: 1998 UNTIL : 2001

AMMOUNT FUNDED: 15.000.000 pta

PROJECT LEADER: Dr. Antonio Aguilar Navarro

TITLE OF THE PROJECT : **Dinámica de reacciones elementales entre neutros y entre iones y moléculas: Experimentos con haces moleculares y métodos teóricos.**

PROGRAMME: Promoción General del Conocimiento, Plan Nacional de Investigación Científica, Desarrollo e Innovación Tecnológico (2000-2003) (PROJECT: BQU2001-3018)

DURATION FROM: 2001 UNTIL: 2004

AMMOUNT FUNDED: 171.228,37 €

PROJECT LEADER: Dr. Antonio Aguilar Navarro

TITLE OF THE PROJECT: **Cinética y dinámica de reacciones bimoleculares de relevancia en química atmosférica y en procesos de combustión**

PROGRAMME: Promoción General del Conocimiento (Proyecto PB98-1209-C02-01 (subproyecto de proyecto coordinat))

DURATION FROM: 1999 UNTIL : 2002

AMMOUNT FUNDED: 48.081 €

PROJECT LEADER: Dr. Miguel González Pérez (IP subproyecto 1 i coordinador)

TITLE OF THE PROJECT: **Estudio teórico y experimental de la cinética y dinámica de reacciones químicas. Química Atmosférica, procesos de combustión y primeras aplicaciones a sistemas con un número elevado de átomos.**

PROGRAMME: Promoción General del Conocimiento (Proyecto BQU2002-04269-C02-02 (subproyecto de proyecto coordinat))

DURATION FROM: 2002 UNTIL : 2005

AMMOUNT FUNDED: 74.510 €

PROJECT LEADER: Dr. Miguel González Pérez (IP subproyecto 2 i coordinador)

TITLE OF THE PROJECT: **Dinámica y cinética de reacciones químicas en superficies: modelación y simulación de la catálisis heterogénea desde primeros principios**

PROGRAMME: Promoción General del Conocimiento (Proyecto BQU2002-03351)

DURATION FROM: 2002 UNTIL : 2005

AMMOUNT FUNDED: 32.200 €

PROJECT LEADER: Dr. Ramón Sayós Ortega

PROJECT TITLE : **Fisicoquímica de la disponibilidad de metales pesados en sistemas macromoleculares naturales**

PROGRAMME: Promoción General del Conocimiento, Plan Nacional de Investigación Científica, Desarrollo e Innovación Tecnológico (Proyecto: BQU2003-09698-C02-02)

DURATION FROM: 2004 UNTIL A: 2006

AMMOUNT FUNDED: 32.000 €

PROJECT LEADER: Dr. Francesc Mas Pujadas

TITLE OF THE PROJECT: **Arquitectura de cristales, interacciones magnéticas y enlace: estudio teórico y estructural**

PROGRAMME: DGEIC (PB98-1166-C02-01)

DURATION FROM: 1999 UNTIL: 2002
AMMOUNT FUNDED: 13.000.000 pts
PROJECT LEADER: Dr. Santiago Alvarez Reverter i Dr. Juan J. Novoa Vide

TITLE OF THE PROJECT: **Estructura electrónica y propiedades de moléculas y sólidos inorgánicos**

PROGRAMME: Promoción General del Conocimiento (Proyecto BQU2002-04033)
DURATION FROM: 2002 UNTIL : 2005
AMMOUNT FUNDED: 149.300 €
PROJECT LEADER: Dr. Santiago Alvarez Reverter i Dr.Pere Alemany Cahner

TITLE OF THE PROJECT: **Arquitectura y dinámica de cristales moleculares magnéticos**

PROGRAMME: Promoción General del Conocimiento (Proyecto BQU2002-04587-C02-02)
DURATION FROM: 2002 UNTIL : 2005
AMMOUNT FUNDED: 90.000 €
PROJECT LEADER: Dr. Juan J. Novoa Vide

TITLE OF THE PROJECT: **Predicción ab initio de parámetros derivados de la estructura electrónica en Química de Materiales. Un punto de partida para la simulación no empírica de propiedades macroscópicas.**

PROGRAMME: Promoción General del Conocimiento (Proyecto BQU2002-04029-C02-01)
DURATION FROM: 2002 UNTIL : 2005
AMMOUNT FUNDED: 107.000 €
PROJECT LEADER: Dr. Francesc Illas i Riera

TITLE OF THE PROJECT: **Estudio teórico de mecanismos de reacción de interés en química atmosférica**

PROGRAMME: Promoción General del Conocimiento (Proyecto PB98-1240-CO2-01)
DURATION FROM: 1999 UNTIL : 2002
AMMOUNT FUNDED: 41.469,84 €
PROJECT LEADER : Dr. Santiago Olivella Nello

TITLE OF THE PROJECT: **Estudio teórico de reacciones de oxidación de interés en la Química de la Troposfera**

PROGRAMME: Promoción General del Conocimiento (Proyecto BQU2002-04485-CO2-02)
DURATION FROM: 2002 UNTIL : 2005
AMMOUNT FUNDED: 23.350,00 €
PROJECT LEADER : Dr. Albert Solé Sabaté

TITLE OF THE PROJECT: **Estudio teórico de la estructura y la dinámica de sistemas moleculares complejos: reacciones orgánicas, motores moleculares y sistemas bioorgánicos**

PROGRAMME: Promoción General del Conocimiento (Proyecto BQU2002-00293)
DURATION FROM: 1 de November, 2002 UNTIL : 31 d'October de 2005
AMMOUNT FUNDED: 27.700,00 €
PROJECT LEADER: Dr. Josep Maria Bofill Villà

Integrated Actions

PROJECT TITLE: Desarrollo y puesta a punto de un sistema de guía de iones octupolar para la generación de haces moleculares iónicos de baja energía. estudio de reacciones ion-molécula.

PROGRAMME: Acciones Integradas (entre Spain y la República Italiana)

FUNDED BY: Ministerio de Ciencia y Tecnología (Ref.HI2001-0050)

FROM/TO: 2002 / 2003

AMMOUNT FUNDED: 8.474,28 €

PROJECT LEADER: Dr. Antonio Aguilar Navarro

PROJECT TITLE: Modelización teórica ab initio del magnetismo en compuestos laminares del tipo $\text{Cu}(\text{OH})_3\text{X}$

PROGRAMME: Acción integrada Hispano-Francesa HF2000-0052

FUNDED BY: Ministerio de Ciencia y Tecnología

DURATION FROM: 2001 UNTIL: 2002

AMMOUNT FUNDED: 800.000 pts

PROJECT LEADER: Dr. Juan J. Novoa Vide

PROJECT TITLE: Ingeniería de cristales moleculares iónicos de interés tecnológico. Naturaleza de sus interacciones A-H...B

PROGRAMME: Acción integrada Hispano-Italiana HI2000-0056

FUNDED BY: Ministerio de Ciencia y Tecnología

DURATION FROM: 2001 UNTIL: 2002

AMMOUNT FUNDED: 960.000 €

PROJECT LEADER: Dr. Juan J. Novoa Vide

PROJECT TITLE: Agregados metálicos soportados en óxidos: Estructura, enlace y reactividad

PROGRAMME: Acciones Integradas Hispano-Alemanas (Proyecto: HA2000-0001)

FUNDED BY: Ministerio de Ciencia y Cultura

DURATION FROM: 2001 UNTIL: 2002

AMMOUNT FUNDED: 8474 €

PROJECT LEADER: Dr. Francesc Illas i Riera

PROJECT TITLE: Simulación mecano-cuántica de reacciones catalíticas sobre superficies de materiales metálicos y cerámicos.

PROGRAMME: Acciones Integradas Hispano-Italianas (Proyecto: HI2001-0201)

FUNDED BY: Ministerio de Educación y Cultura

DURATION FROM: 2002 UNTIL: 2003

AMMOUNT FUNDED: 8474 €

PROJECT LEADER: Dr. Francesc Illas i Riera

Projectes finançats per la Generalitat de Catalunya (DURSI)

TITLE OF THE PROJECT: Aproximació genética i metabòlica a la optimització de processos de producció de biomolècules d'interès farmacològic o industrial

PROGRAMME: Xarxes temàtiques (Ref. 2000XT-00012)

DURATION FROM: 2001 UNTIL :2003

AMMOUNT FUNDED: 7.200,00 €

PROJECT LEADER: Dra. Marta Cascante Serratosa

TITLE OF THE PROJECT: Grup de Bioquímica Integrativa

PROGRAMME: Projectes de recerca per potenciar els grups de recerca consolidats (Ref. 2001SGR00111)

DURATION FROM: 2001 UNTIL :2005

AMMOUNT FUNDED: 31.252,63 €

PROJECT LEADER: Dra. Marta Cascante Serratosa

TITLE OF THE PROJECT: Proyecto de Cooperación con la Universidad de California (Harbor-UCLA Medical School)

PROGRAMME: Ajudes a la Investigació (Ref. 2001AGP)

DURATION FROM: 2002 UNTIL :2003

AMMOUNT FUNDED: 3.006,00 €

PROJECT LEADER: Dra. Marta Cascante Serratosa

TITLE OF THE PROJECT: Acción Integrada con el Centre National de la Recherche Scientifique

PROGRAMME: Ajudes a la Investigació (Ref. ABM/acs/ACI2002-19)

DURATION FROM: 2002 UNTIL :2003

AMMOUNT FUNDED: 4.500,00 €

PROJECT LEADER: Dr. Josep J Centelles

TITLE OF THE PROJECT: Acción Integrada con la Región de Aquitania

PROGRAMME: Ajudes a la Investigació (Ref. ABM/acs/ACI2002-18)

DURATION FROM: 2002 UNTIL :2003

AMMOUNT FUNDED: 4.000,00 €

PROJECT LEADER: Dra. Marta Cascante Serratosa

TITLE OF THE PROJECT: Aproximació genética i metabòlica a la optimització de processos de producció de biomolècules d'interès farmacològic o industrial.

PROGRAMME: Xarxes temàtiques (Ref. 2002XT-00012)

DURATION FROM: 2002 UNTIL :2003

AMMOUNT FUNDED: 8.550,00 €

PROJECT LEADER: Dra. Marta Cascante Serratosa

TITLE OF THE PROJECT: Cinética i Dinàmica de les Reaccions Elementals

PROGRAMME: II Pla de Recerca de Catalunya. Grups de Recerca Consolidats (projecte 1998SGR00008)

DURATION FROM: 1998 UNTIL : 2000

AMMOUNT FUNDED: 2.500.000 pta

PROJECT LEADER:Dr. Antonio Aguilar Navarro

TITLE OF THE PROJECT: **Xarxa de Química Teòrica**
PROGRAMME: II Pla de Recerca de Catalunya (Ref. 2000XT 00039)
DURATION FROM: 2001 UNTIL : 2002
AMMOUNT FUNDED: 1.200.000 pta
PROJECT LEADER: Dr. Antonio Aguilar Navarro

TITLE OF THE PROJECT: **Cinètica i Dinàmica de les Reaccions Elementals**
PROGRAMME: II Pla de Recerca de Catalunya. Grups de Recerca Consolidats (projecte 2000SGR 00016)
DURATION FROM: 2000 UNTIL : 2002
AMMOUNT FUNDED: 3.600.000 pta
PROJECT LEADER: Dr. Antonio Aguilar Navarro

PROJECT TITLE: **Cinètica i Dinàmica de les Reaccions Elementals.**
PROGRAMME: III Pla de Recerca de Catalunya. Grups de Recerca Consolidats (Ref. 2001SGR 00041)
DURATION FROM: 2001 UNTIL A 2004
AMMOUNT FUNDED: 34.858,70 €
PROJECT LEADER: Dr. Antonio Aguilar Navarro

PROJECT TITLE: **Aplicacions dels làsers en Química**
PROGRAMME: Xarxes Temàtiques (Ref. 1999XT 00006)
DURATION FROM: 9/2/2000 UNTIL 31/2/2001
AMMOUNT FUNDED: 7813 €
PROJECT LEADER: Dr. Miguel González Pérez

PROJECT TITLE: **Aplicacions dels làsers en Química**
PROGRAMME: Xarxes Temàtiques (Ref. 2001XT 00006)
DURATION FROM: 1/1/2002 UNTIL 31/12/2003
AMMOUNT FUNDED: 7813 €
PROJECT LEADER: Dr. Miguel González Pérez

PROJECT TITLE: **Aplicacions dels làsers en Química**
PROGRAMME: Xarxes Temàtiques (Ref. 2003XT 00068)
DURATION FROM: 2/7/2003 UNTIL 2/7/2005
AMMOUNT FUNDED: 8200 €
PROJECT LEADER: Miguel González Pérez

PROJECT TITLE: **Fisicoquímica de Sistemes Macromoleculars o Col·loïdals d'Interès Ambiental**
PROGRAMME: Ajuts per als projectes de recerca de Catalunya (Ref. 2001SGR 00301)
DURATION FROM: 2002 UNTIL A 2004
AMMOUNT FUNDED: 15.025,30 €
PROJECT LEADER: Dr. Jaume Puy Llorens

PROJECT TITLE: **Fisicoquímica de Sistemes Macromoleculars o Col·loïdals d'Interès Ambiental**
PROGRAMME: Ajuts per als projectes de recerca de Catalunya (Ref. 1999SGR 00177)
DURATION FROM: 2000 UNTIL A 2001

AMMOUNT FUNDED: 2.400.000 ptes
PROJECT LEADER: Dr. Jaume Puy Llorens

PROGRAMME: **Ajuts a Grups de Recerca Consolidats.**
PROJECT: 1999SGR-0046
DURATION FROM: 2000 UNTIL: 2002
AMMOUNT FUNDED: 2.700.000 Pts
PROJECT LEADER: Dr. Juan J. Novoa Vide

PROGRAMME: **Ajuts a Grups de Recerca Consolidats**
PROJECT: 2001SGR-0044
DURATION FROM: 2002 UNTIL: 2005
AMMOUNT FUNDED: 46.879 €
PROJECT LEADER: Dr. Juan J. Novoa Vide

PROGRAMME: **Ajuts a Grups de Recerca Consolidats**
PROJECT: 2001SGR0043
DURATION FROM: 2001 UNTIL : 2004
AMMOUNT FUNDED: 42.070,85 €
PROJECT LEADER: Dr. Francesc Illas i Riera

PROGRAMME: **Ajuts a Grups de Recerca Consolidats**
PROJECT: 2001SGR0048
DURATION FROM: 1 de January, 2001 UNTIL : 31 de December de 2004
AMMOUNT FUNDED: 39.065,79 €
PROJECT LEADER: Dr. Santiago Olivella Nello

PROGRAMME: **Accions especials, ACES2003**
PROJECT: Potenciació i Internacionalització de les activitats del Centre especial de Recerca en Química Teòrica
DURATION FROM: 2004 UNTIL : 2005
AMMOUNT FUNDED: 24.000 €
PROJECT LEADER: Dr. Francesc Illas i Riera

Projects funded by the European Union

TITLE OF THE PROJECT: Towards european neuronal cell stimulation

PROGRAMME: Ayudas a la Investigación FP6-2002-LifeSciHealth

DURATION FROM : 2003 UNTIL : 2006

AMMOUNT FUNDED: 200.000,00 €

PROJECT LEADER : Dra. Marta Cascante Serratos

TITLE OF THE PROJECT: Quantum and semiclassical computational techniques for intra and intermolecular reaction dynamics of polyatomic systems, including solvent effects.

PROGRAMME: COST Action D9 (D9/0008/98)

DURATION FROM: 1998 UNTIL : 2003

PROJECT LEADER : Dr. Antonio Aguilar Navarro

TITLE OF THE PROJECT: METACHEM: Metalaboratories for Complex Computational Applications in Chemistry

PROGRAMME: COST Action D23 (D23/2000)

DURATION FROM: 2000 UNTIL : 2005

PROJECT LEADER: Dr. Antonio Aguilar Navarro

TITLE OF THE PROJECT: Physico-chemical processes in hyperenthalpic hypersonic reactive and multitemperature CO₂-N₂ gas flows

PROGRAMME: INTAS Ref. INTAS-99-00701(projecte coordinat)

DURATION FROM: 1-5-2000 UNTIL 1-5-2002

AMMOUNT FUNDED: 12.000 €

PROJECT LEADER: Dr. Ramón Sayós Ortega

TITLE OF THE PROJECT: Sensor development for routine prediction of metal biouptake in freshwaters and soil solutions (BIOSPEC)

PROGRAMME: Preserving the Ecosystem: environmental research, Commission Europeene (DG-RTD) EVK1-CT2001-00086

DURATION FROM: 2001 UNTIL : 2004

AMMOUNT FUNDED: 189.478 €

PROJECT LEADER: Dr. Jaume Puy Llorens

TITLE OF THE PROJECT: Understanding and prediction of magnetic properties in molecules and solids

PROGRAMME: COST Action D26 (D9/0008/98)

DURATION FROM: 2003 UNTIL : 2006

AMMOUNT FUNDED:

PROJECT LEADER: Dr. Francesc Illas i Riera

TITLE OF THE PROJECT: Supramolecular networks

PROGRAMME: COST D11-0017-9

FUNDED BY: Unió Europea

DURATION FROM: 2000 UNTIL: 2004

AMMOUNT FUNDED:-

PROJECT LEADER: Dr. Juan J. Novoa Vide

Projects funded by the Universitat de Barcelona

PROGRAMME: **Ajuts de la UB per accés dels grups del CeRQT a recursos de Supercomputació**

DURATION FROM: 2001 UNTIL: 2003

AMMOUNT FUNDED: 39.000 €

PROJECT TITLE: **Biofísica de las interacciones biopolímero-disolución y su efecto en el metabolismo celular**

PROGRAMME: PROGRAMME Sócrates de cooperación con América Latina (Argentina)

DURATION FROM: 2002 UNTIL: 2002

AMMOUNT FUNDED: 1.803,04 €

PROJECT LEADER: Dr. Francesc Mas Pujadas

Other sources of funding

PROJECT TITLE: **Explotación de las diferencias metabólicas entre las células normal y tumoral en la búsqueda de nuevas dianas antitumorales.**

PROGRAMME: Ayudas a la Investigación ONO3-70-0

FUNDED BY: Fundació Caixa de Pensions 'La Caixa'

DURATION FROM: 2003 UNTIL: 2005

AMMOUNT FUNDED: 83.000,00 €

PROJECT LEADER: Dra. Marta Cascante Serratosa

TITLE OF THE PROJECT: **Cinética y Dinámica de Reacciones Elementales**

PROGRAMME: Profesores Visitantes Iberdrola Ciencia y Tecnología

FUNDED BY : IBERDROLA, S.A.

DURATION FROM: 1998 UNTIL : 2001

AMMOUNT FUNDED: 1.000.000 pta

PROJECT LEADER: Dr. Antonio Aguilar Navarro

PROJECT TITLE: **Ayuda del PROGRAMME “Profesores Visitantes IBERDROLA Ciencia y Tecnología”**

PROGRAMME: Profesores Visitantes IBERDROLA Ciencia y Tecnología

FUNDED BY: IBERDROLA, SA

DURATION FROM: 2001 UNTIL: 2003

AMMOUNT FUNDED: 45.000.000 pts.

PROJECT LEADER: Dr. Juan J. Novoa Vide

Doctoral Thesis by member of the CeRQT defended during 2001-2003

1) **Antonio Rodríguez-Forte**: “Predicció de constants d'acoblament magnètic en compostos dinuclears de metalls de transició”. Universitat de Barcelona, January 2001. Supervisor: Pere Alemany.

2) **Maria Teresa García Hernández**: “Determinación teórica de la estructura, mecanismo de enlace y modos normales de vibración de especies adsorbidas en superficies y electrodos de platino”, Universitat de Barcelona, March 2001, Supervisor: Francesc Illas.

3) **Iberio de Pinho Ribeiro Moreira**: “Título: Modelos mecanocuánticos para la determinación precisa de constantes de acoplamiento magnético en sólidos iónicos”, Universitat de Barcelona, March 2001, Supervisor: Francesc Illas.

4) **Rosendo Valero Montero**: “Ab initio study of the $O(^1D)$, $O(^3P) + N_2O$ and $N(^2D) + NO$ reactions of interest in atmospheric chemistry and combustion processes”. Universitat de Barcelona, June 2001. Supervisors: Miguel González i Ramón Sayós

5) **Ana A. Palacios Ruiz**: “Interacciones metal-metal en compuestos dinucleares y de alta dimensionalidad”. Universitat de Barcelona, October 2001. Supervisors: Santiago Alvarez i Pere Alemany

6) **Carolina Oliva García** : “De la estructura electrónica a la dinámica de reacciones. Estudio teórico de los sistemas $O(^3P, ^1D) + H_2O$ y $N(^4S) + O_2$ ”. Universitat de Barcelona, November 2001. Supervisors: Ramón Sayós i Miguel González

7) **Irene Miquel Plana**: “The atmospheric reaction of the excited nitrogen atom with molecular oxygen: ab initio study of the potential energy surface and classical and quantum dynamics”, Universitat de Barcelona, June 2002. Supervisors: Miguel González i Ramón Sayós

8) **Sergio Madurga Díez**: “Efecto de las fuerzas de polarización sobre los equilibrios conformacionales en disolución”, Universidad: Barcelona, July 2003, Supervisor: Eudald Vilaseca.

9) **David Domínguez Ariza**: “Estudio teórico de estados excitados en superficies y sólidos”, Universidad: Barcelona, Decembre 2003, Supervisors: Carme Sousa i Francesc Illas