

Electronic Structure: Principles and Applications ESPA 2008

*Universitat de les Illes Balears
2-5 September 2008
Palma de Mallorca*



Tuesday 2 September

16:00 – 19:00 Registration *Sa Riera Building (C/ Miquel dels Sants, 2. Palma)*
20:00 Welcome Reception *Castell de Bellver*

Wednesday 3 September (*Gaspar Melchor de Jovellanos Building. Universitat de les Illes Balears. Cra. Valldemossa km 7.5*)

08:30-09:00 *Registration*

Session A. Chair: Juan Bertrán, *Universitat Autònoma de Barcelona*

09:00-09:40 *Plenary Lecture PL1*

Gustavo E. Scuseria. *Rice University, USA*

“Range Separation, Local Hybridization and their combination for improving density functionals”

09:40-10:20 *Plenary Lecture PL2*

António J.C. Varandas. *Universidade de Coimbra, Portugal*

“Scaling and Extrapolation of conventional ab initio energies: clues to accurate potentials”

10:20-10:40 *Oral Presentation OP1*

Rita Prosmi. *Instituto de Física Fundamental (IFF-CSIC), Spain*

“Ab initio intermolecular potentials and vibrational dynamics of Rg₂-dihalogen clusters”

10:40-11:00 *Oral Presentation OP2*

Miquel Solà. *Universitat de Girona, Spain*

“Recent advances in the quantification of aromaticity from electronic delocalization measures”

11:00-11:30 *Coffee Break*

Session B. Chair: Jesús Ugalde, *Euskal Herriko Unibertsitatea*

11:30-12:10 *Plenary Lecture PL3*

Tom Ziegler. *University of Calgary, Canada*

“Beating the heavy metal blues with DFT. First Principle calculations of NMR, ESR, CD and MCD parameters of heavy metal complexes”

12:10-12:30 *Oral Presentation OP3*

Florentino Borondo. *Universidad Autónoma de Madrid, Spain*

“The geometry of the transition state for the LiNC=LiCN isomerization reaction”

12:30-12:50 *Oral Presentation OP4*

Miquel Torrent-Sucarrat. *Vrije Universiteit Brussel, Belgium*

“New insights in the density functional theory based reactivity descriptors”

12:50-13:10 *Oral Presentation OP5*

Coen de Graaf. *Universitat Rovira i Virgili, Spain*

“Ab initio study of the light-induced excited state spin trapping (LIESST) in Fe and Co complexes”

13:10-13:30 *Oral Presentation OP6*

Oleg Poleshchuk. *Tomsk State Pedagogical University, Russia*

“DFT Study of structure, stability and hyperfine interactions of halogen and SO₃ complexes”

13:30-15:30 *Lunch. Gaspar Mechor de Jovellanos Building*

Session C. Chair: José Angel Sordo, *Universidad de Oviedo*

15:30-16:10 *Plenary Lecture PL4*

Orlando Tapia. *Uppsala University, Sweden*

“Linear Superposition principle: Towards a quantum theory of chemical processes”

16:10-16:30 *Oral Presentation OP7*

David Quiñonero. *Universitat de les Illes Balears, Spain*

“A novel anion- π interaction in biological systems: interplay between anion- π and C-H/ π interactions”

16:30-16:50 *Oral Presentation OP8*
Tanja van Mourik. *University of St Andrews, UK*
“Assessment of density functionals for intramolecular dispersion-rich interactions”

16:50-17:30 *Plenary Lecture PL5*
Berta Fernández. *Universidad de Santiago de Compostela, Spain*
“Van der Waals complexes: Accurate evaluation of interaction properties”

17:30-19:30 *Poster Session*

Thursday 4 September (*Gaspar Melchor de Jovellanos Building. Universitat de les Illes Balears. Cra. Valldemossa km 7.5*)

Session D. Chair: Miquel Duran, *Universitat de Girona*

09:00-09:40 *Plenary Lecture PL6*
Christopher J. Cramer. *University of Minnesota, USA.*
“Electronic structure challenges associated with dioxygen activation at mono- and binuclear copper enzyme site models”

09:40-10:20 *Plenary Lecture PL7*
Maria João Ramos. *Universidade do Porto, Portugal*
“Computational Enzymology and Drug Design”

10:20-10:40 *Oral Presentation OP9*
José Manuel Martínez. *Universidad de Sevilla, Spain*
“Combining molecular dynamics simulations and X-Ray absorption spectroscopy: from aqueous to biological cation environments”

10:40-11:00 *Oral Presentation OP10*
Ellie L. Uzunova. *Bulgarian Academy of Sciences, Bulgaria*
“Theoretical study of transition metal cation exchanged zeolites: Interaction with NO”

11:00-11:30 *Coffee Break*

Session E. Chair: Enrique Sánchez Marcos, *Universidad de Sevilla*

11:30-12:10 *Plenary Lecture PL8*

Victor Guallar. *Barcelona Supercomputing Center, Spain*
“QM/MM Studies of electron transfer in cytochromes”

12:10-12:50 *Plenary Lecture PL9*

Dimas Suárez. *Universidad de Oviedo, Spain*
“Structure, dynamics and catalysis of matrix metalloproteinases: A computational study”

12:50-13:10 *Oral Presentation OP11*

Josep M. Oliva. *Instituto de Química-Física Rocasolano - CSIC, Spain*
“On the electronic structure of dianions, radical anions and diradicals derived from carborane dimers”

13:10-13:30 *Oral Presentation OP12*

Silvia Ferrer. *Institut de Génétique et de Biologie Moléculaire et Cellulaire (IGBMC), France*
“Theoretical Studies of human nuclear receptor PPAR γ ”

13:30-15:30 *Lunch. Gaspar Mechor de Jovellanos Building*

15:30 *Visit to “Coves del Drac”*

21:00 *Dinner. Gran Restaurant Casino de Mallorca*

Friday 5 September (*Gaspar Melchor de Jovellanos Building. Universitat de les Illes Balears. Cra. Valldemossa km 7.5*)

Session F. Chair: Angels González Lafont, *Universitat Autònoma de Barcelona*

09:00-09:40 *Plenary Lecture PL10*

Marco Antonio Chaer Nascimento. *Instituto de Química da UFRJ, Brazil*
“The nature of the chemical bond”

09:40-10:20 *Plenary Lecture PL11*

Paolo Carloni. *Internazionali Superiore di Studi Avanzati (SISSA), Italy*
“Hybrid Car-Parrinello/Molecular Mechanics calculations of metal-based systems of pharmaceutical relevance”

10:20-10:40 *Oral Presentation OP13*
Cristina Díaz. *Universidad Autónoma de Madrid, Spain*
“A theoretical study of physisorption of molecular hydrogen on metal-organic framework materials”

10:40-11:00 *Oral Presentation OP14*
Ameya Joshi. *Corning Incorporated, USA*
“Density functional theory (DFT) study of the interaction of ammonia with pure and tungsten-doped ceria”

11:00-11:30 *Coffee Break*

Session G. Chair: Alfonso Hernández-Laguna, *Estación Experimental del Zaidín, CSIC- Granada*

11:30-12:10 *Plenary Lecture PL12*
Iñaki Tuñón. *Universidad de Valencia, Spain*
“How does protein dynamic influence the rate of enzymatic reactions? The case of Chalcone Isomerase”

12:10-12:50 *Plenary Lecture PL13*
Manuel F. Ruiz-López. *Université Henry Poincaré, France*
“Chemical reactions in molecular vessels: Insights from computational studies”

12:50-13:10 *Oral Presentation OP15*
J. Raúl Alvarez-Idaboy. *Universidad Nacional Autónoma de México, Mexico*
“The mechanism of the Baeyer-Villiger reaction: Quantum Chemistry and TST study supported by experimental kinetic data”

13:10-13:30 *Oral Presentation OP16*
Valery I. Poltev. *Universidad Autónoma de Puebla, Mexico and Institute of Theoretical and Experimental Biophysics RAS, Russia*
“DFT Study of minimal fragments of nucleic acid single chain for explication of sequence dependence of DNA duplex conformation”

13:30-15:30 *Lunch. Gaspar Mechor de Jovellanos Building*

Session H. Chair: Manuel Yañez, *Universidad Autónoma de Madrid*

15:30-15:50 *Oral Presentation OP17*

Laura Gagliardi. *Université de Genève, Switzerland*
“Recent advances in metal metal multiple bonding”

15:50-16:10 *Oral Presentation OP18*

Carles Bo. *Institute of Chemical Research of Catalonia (ICIQ) and Universitat Rovira i Virgili, Spain*
“Multi-step modeling of giant polyoxometalates: Dynamic structure of encapsulated water clusters”

16:10-16:50 *Plenary Lecture PL14*

Juan J. Novoa. *Universidad de Barcelona, Spain*
“The nature of long-distance bonds ($\sim 3 \text{ \AA}$) in crystals and solution”

17:30-19:30 *Guided visit to Palma*

21:30 *Closing Banquet. Restaurante Mediterráneo, Paseo Marítimo, 33, 5th floor.*