SANTIAGO DE COMPOSTELA 2011

Ninth triennial congress of the

WORLD ASSOCIATION OF THEORETICAL AND COMPUTATIONAL CHEMISTS

Santiago de Compostela (Spain)
17-22 July, 2011

POCKET PROGRAMME

SUNDAY JULY 17	**AUDITORIO DE GALICIA**
11.00-12.30	S1.1 **Opening Ceremony**
11.00-11.45	"GALICIA WELCOMES YOU"
11.45-12.30	OFFICIAL OPENING OF THE CONFERENCE
12.30-13.10	S2.1 **Plenary Session (Chair: *Peter Pulay*)**
13.10-15.30	LUNCH BREAK
15.30-17.30	**Poster Session I** (PI-1 to PI-283) **FACULTY OF ECONOMY**
17.40-19.00	S3.1 **Plenary Session (Chair: *Francesc Illas*)**
19.00-21.00	**WELCOME MIXER**

MONDAY JULY 18	**FACULTY OF MEDICINE**				
	ROOM A (AULA 4)	**ROOM B (AULA 5)**	**ROOM C (AULA 7)**	**ROOM D (AULA 8)**	**ROOM E (SALÓN DE ACTOS)**
9.00-10.30	**M1.1** Theory I. Symposium in Honor of Klaus Ruedenberg (Chair: *Miroslav Urban*)	**M1.2** Relativistic effects (Chair: *Colin Marsden*)	**M1.3** Electrochemical/ optical properties (Chair: *M. Verónica Ganduglia-Pirovano)*	**M1.4** Radical reactions (Chair: *Daniel M. Chipman*)	**M1.5** Simulations of biochemical systems (Chair: *Laurence Leherte*)
10.30-11.00	COFFEE BREAK				

MONDAY JULY 18 **FACULTY OF MEDICINE**

	ROOM A (AULA 4)	ROOM B (AULA 5)	ROOM C (AULA 7)	ROOM D (AULA 8)	ROOM E (SALÓN DE ACTOS)
11.00-13.00	**M2.1** New developments in CC theory (Chair: *Geza Fogarasi*)	**M2.2** Molecular Rotation and vibration (Chair: *Chaoyuan Zhu*)	**M2.3** Heterogeneous Catalysis (Chair: *Paola Belanzoni*)	**M2.5** Enzymatic Catalysis. Symposium in Honor of Joan Bertran (Chair: *Enrique Sánchez- Marcos*)	**M2.4** Hydrogen bonds/ Non-covalent Interactions (Chair: *Sławomir Grabowski*)
13.00-15.30	LUNCH BREAK				
15.30-17.30	**M3.5** Computational Strategies for biomolecular systems (Chair: *Javier Luque*)	**M3.2** Quantum Montecarlo (Chair: *Bruce Garrett*)	**M3.3** Clusters/ nanostructures I (Chair: *Minh To Nguyen*)	**M3.4** Inorganic photochemistry/ Transition metals (Chair: *Timofei Privalov*)	**M3.1** DFT: New developments/ applications I (Chair: *Clemence Corminboeuf*)
17.30-18.00	COFFEE BREAK				
18.00-19.40	**M4.5** Adsorption/ Surface interactions (Chair: *Lorenzo Maschio*)	**M4.2** Chirality (Chair: *Robert Berger*)	**M4.3** Astrochemistry/ Chemistry of the atmospheres.I (Chair: *Josep M. Anglada*)	**M4.4** Biomolecular Interactions (Chair: *Pedro B. Coto*)	**M4.1** Solvation (Chair: *Kaline Coutinho*)
19.00-19.40			**M4.3.1** More on excited states & spectroscopy		

TUESDAY JULY 19 — AUDITORIO DE GALICIA

9.00-11.00	TU.1. **Plenary Session (Chair: *Enrico Clementi*)**
11.00-11.30	COFFEE BREAK
11.30-13.30	**Poster Session II** (PII-1 to PII-299) **FACULTY OF ECONOMY**
13.30-15.30	**LUNCH BREAK**
16.00	**EXCURSION**

WEDNESDAY JULY 20 — FACULTY OF MEDICINE

	ROOM A (AULA 4)	ROOM B (AULA 5)	ROOM C (AULA 7)	ROOM D (AULA 8)	ROOM E (SALÓN DE ACTOS)
9.00-10.30	**W1.1** Aromaticity (Chair: *Shogo Sakai*)	**W1.5** Non-covalent interactions (Chair: *Takeshi Sato*)	**W1.3** Reaction Mechanisms (Chair: *Devesh Kumar*)	**W1.4** Bond activation reactions (Chair: *Gilles Ohanessian*)	**W1.2** Methodology developments/ large molecules (Chair: *Jan Řezáč*)
10.30-11.00	COFFEE BREAK				
11.00-13.00	**W2.5** Electronic spectra/ one & two photon excitations. Symposium in memoriam of Luis Serrano Andrés (Chair: *Lluis Blancafort*)	**W2.2** Explicitly correlated methods/ Choleski decomposition (Chair: *Sergei Gusarov*)	**W2.3** Functional materials (Chair: *Carmen J. Calzado*)	**W2.4** Porous materials/gas storage (Chair: *Andriy Kovalenko*)	**W2.1** DFT: New developments/ applications II (Chair: *Suehiro Iwata*)

WEDNESDAY JULY 20 **FACULTY OF MEDICINE**

	ROOM A (AULA 4)	ROOM B (AULA 5)	ROOM C (AULA 7)	ROOM D (AULA 8)	ROOM E (SALÓN DE ACTOS)
13.00-15.30	LUNCH BREAK				
15.30-17.30	**W3.1** Theory II (Chair: *Gregory S. Tschumper*)	**W3.2** Photodynamic simulations (Chair: *Mario Barbatti*)	**W3.3** VB theory (Chair: *David Danovich*)	**W3.4** Clusters/ Nanostructures II (Chair: *Rafael Escribano*)	**W3.5** Organic reaction mechanisms (Chair: *Evgenyi Gromov*)
17.30-18.00	COFFEE BREAK				
18.00-19.40	**W4.1** Relativistic effects. II (Chair: *Robert Ponec*)	**W4.2** Quantum Chemical topology (Chair: *Peeter Burk*)	**W4.3** Correlation & molecular properties/ dispersion (Chair: *Rosa Caballol*)	**W4.5** Astrochemistry/ Chemistry of the atmospheres. II (Chair: *Marzio Rosi*)	**W4.4** Biomolecular Interactions/ Proton and electron transfer. Symposium in Memoriam of Zvonko Maksic (Chair: *David Smith*)
19.00-19.40	**W4.1.1** More on catalysis	**W4.2.1**. Reactivity		**W4.5.1**. More on solvation	
21.30	CONCERT AT THE CATHEDRAL				

THURSDAY JULY 21 **FACULTY OF MEDICINE**

	ROOM A (AULA 4)	ROOM B (AULA 5)	ROOM C (AULA 7)	ROOM D (AULA 8)	ROOM E (SALÓN DE ACTOS)
9.00-11.10	**TH1.5** Metalloproteins/ Alzheimer dissease (Chair: *Valérie Brenner*)	**TH1.2** Force fields/ Free energy landscapes (Chair: *Jiali Gao*)	**TH1.3** Molecular devices/ self assembling (Chair: *Christian van Alsenoy*)	**TH1.4** Excited states in biomolecules (Chair: *Adelia Aquino*)	**TH1.1** Electron correlation theory / linear scaling (Chair: *Anthony D. Dutoi*)
11.10-11.40	COFFEE BREAK				
12.00	**BOTAFUMEIRO EXHIBITION AT THE CATHEDRAL**				
13.00-15.30	LUNCH BREAK				
15.30-17.10	**TH2.1** GPU Technology (Chair: *Jiří Pittner*)	**TH2.2** Chemical dynamics/ reaction pathways (Chair: *Antonio Laganà*)	**TH2.3** Nanostructures (Chair: *Fernando Martín*)	**TH2.4** Organometallic chemistry / homogeneous catalysis (Chair: *Agustí Lledós*)	**TH2.5** Cycloadditions (Chair: *Angels González Lafont*)
17.10-17.40	COFFEE BREAK				
17.40-19.30	**TH3.1** Ring Currents/ magnetism/NMR (Chair: *Gabriela Borosky*)	**TH3.2** Molecular Recognition/ isomerization in biomolecules (Chair: *Pedro A. Fernandes*)	**TH3.5** Enzymatic Reactions (Chair: *Juan Frau*)	**TH3.4** Metallochemistry/ more on homogeneous catalysis (Chair: *Feliu Maseras*)	**TH3.3** Molecular Modeling/ Design/ simulations (Chair: *Meredith JT Jordan*)

FRIDAY JULY 22	
9.00-11.00	F1. **Plenary Session (Chair: *Odile Eisenstein*)** **AUDITORIO DE GALICIA**
11.00-11.30	COFFEE BREAK
11.30-13.30	Poster Session III (PIII-1 to PIII-267) **FACULTY OF ECONOMY**
13.30-15.30	**LUNCH BREAK**
15.30-17.30	F2. **Plenary Session (Chair: *Kangnian Fan*)** **AUDITORIO DE GALICIA**
17.30-18.00	**F3.** *Closing Ceremony*
21.00	**BANQUET Pazo de San Lorenzo**

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SUNDAY JULY 17

11.00-12.30	S1.1 **Opening Ceremony** **AUDITORIO DE GALICIA**
11.00-11.45	"GALICIA WELCOMES YOU"
11.45-12.30	OFFICIAL OPENING OF THE CONFERENCE
12.30-13.10	S2.1 **Plenary Session (Chair: Peter Pulay)**
12.30-13.10	**PL1**. **Anne McCoy**. Decoding vibrational spectra in protonated and hydrogen bonded systems
13.10-15.30	LUNCH BREAK
15.30-17.30	**Poster Session I** (PI-1 to PI-283) **FACULTY OF ECONOMY**
17.40-19.00	S3.1 **Plenary Session (Chair: Francesc Illas)**
17.40-18.20	**PL2. Gernot Frenking.** The Chemistry of Carbones CL_2 and Heavier Homologues EL_2 (E = Si – Pb) and the Extension to Group-13 and Group-15 analogues
18.20-19.00	**PL3. Jens Norskov**. Tailoring Surface Chemical Properties Using Electronic Structure Theory
19.00-21.00	**WELCOME MIXER**

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MONDAY JULY 18 **FACULTY OF MEDICINE**

	ROOM A (AULA 4)	ROOM B (AULA 5)	ROOM C (AULA 7)	ROOM D (AULA 8)	ROOM E (SALÓN DE ACTOS)
9.00-10.30	**M1.1** Theory I. Symposium in Honor of Klaus Ruedenberg (Chair: *Miroslav Urban*)	**M1.2** Relativistic effects (Chair: *Colin Marsden*)	**M1.3** Electrochemical/ optical properties (Chair: *M. Verónica Ganduglia-Pirovano*)	**M1.4** Radical reactions (Chair: *Daniel M. Chipman*)	**M1.5** Simulations of biochemical systems (Chair: *Laurence Leherte*)
9.00-9.20	**IL1.** *Henry F. Schaefer* Quantum Chemistry: 1950-1960	**IL2.** *Dieter Cremer* Development And Application Of Analytical Energy Gradients For The NESC (normalized elimination of the small component) method	**IL3.** *Massimilano Aschi* Modelling electrochemical properties in complex molecular systems	**IL4.** *Leo Radom* Hydrogen abstraction by chlorine atom from amino acids: the remarkable influence of polar effects on regioselectivity	**IL5.** *Michele Parrinello* The well-tempered ensemble
9.20-9.40	**IL6.** *James Stewart* Past, present, and future of Semiempirical Methods	**IL7.** *Trond Saue* Complex Response in a 4-component relativistic framework	**IL8.** *Allan L.L. East* The Origin of the Conductivity Maximum in Molten Bismuth Chloride	**IL9.** *Barry Carpenter* Oscillatory product ratios in dynamically controlled reactions	**IL10.** *Pavel Hobza* Design and application of a novel semiempirical QM scoring function

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MONDAY JULY 18 FACULTY OF MEDICINE

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9.40-10.00	**IL11.** *Petr Carsky* Prospects of using mixed plane-wave and Gaussian basis sets in mainstream quantum chemistry	**IL12.** *Sambhu N. Datta* Derivation of relativistic molecular hamiltonian for quantum chemistry	**IL13.** *Georg Schreckenbach* Dye Regeneration Mechanism in the Dye-Sensitized Solar Cell: A Density Functional Study	**IL14.** *Viktorya Aviyente* Understanding the free radical polymerization kinetics with computational tools	**IL15.** *Steven D. Schwartz* Reaction Coordinates in Enzymatic reactions: transition path sampling, the stochastic separatrix, and the reaction coordinate
10.00-10.20	**IL16.** *Ajit J. Thakkar* How Well Are Atomic Correlation Energies Known?	**IL17.** *Gustavo A. Aucar* A full relativistic formalism that gives new insight into magnetic molecular properties	**IL18.** *Elena Bichoutskaia* New theoretical approach to studying the interaction between charged dielectric particles	**IL19.** *Michelle L. Coote* Action at a distance: penultimate unit effects in free-radical polymerization and their implications for modelling radical reactions	**IL20.** *Arieh Warshel* Reference Potentials and CG approaches for simulations of biological systems
10:20-10:30	**OC1.** *Steven Vancoillie* Restricted Multiconfigurational Perturbation Theory Strategies for Transition Metal Systems	**OC2.** *Junji Seino* Two-component relativistic method for large molecular systems	**OC3.** *Gaëtan Bonnard* Structural and electrochemical properties of crystalline para-benzoquinone derivatives from DFT calculations	**OC4.** *Juan Novoa* Unusual long distance cation$^{\delta+\cdots}$ anion$^{\delta-}$ bonding observed in crystals of the TTF$^{\cdot+}$ (tetrathiafulvalene) and TCNE$^{\cdot-}$ (tetracyanoethylene) organic radicals	**OC5.** *Rebeca García-Fandiño* α,γ-peptide nanotubes: a theoretical study

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	ROOM A (AULA 4)	ROOM B (AULA 5)	ROOM C (AULA 7)	ROOM D (AULA 8)	ROOM E (SALÓN DE ACTOS)
10.30-11.00	COFFEE BREAK				
11.00-13.00	**M2.1** New developments in CC theory (Chair: *Geza Fogarasi*)	**M2.2** Molecular Rotation and vibration (Chair: *Chaoyuan Zhu*)	**M2.3** Heterogeneous Catalysis (Chair: *Paola Belanzoni*)	**M2.5** Enzymatic Catalysis. Symposium in Honor of Joan Bertran (Chair: *Enrique Sánchez- Marcos*)	**M2.4** Hydrogen bonds/ Non-covalent Interactions (Chair: *Sławomir Grabowski*)
11.00-11.20	**IL21.** *Martin Head-Gordon* The Coupled Cluster Valence Bond Method: Theory, Implementation and Applications	**IL22.** *Cristina Puzzarini* Puzzling aspects in rotational spectroscopy: when experiment cannot do without theory	**IL23.** *Don G. Truhlar* Density functionals for catalysis	**IL25.** *Sason Shaik* Why does nature use high spin enzymes for bond activation? The concept of exchange-enhanced reactivity	**IL24.** *Tom A. Ford* Molecular complexes – from hydrogen-bonded to van der Waals and back again
11.20-11.40	**IL26.** *Rodney Bartlett* Multi-reference Couple-cluster Theory Made Easy	**IL27**. *Claude Pouchan* Time dependent and time independent methods to compute vibrational spectra	**IL28**. Joerg Meyer 'QM/ME' – a novel embedding approach for adsorbate dynamics on metal surfaces	**IL30**. *Vicent Moliner* Do dynamic or tunneling effects play an important role in enzyme Catalysis? the thymidylate synthase case	**IL29**. *Isabel Rozas* Guanidinium: a versatile cation

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	ROOM A (AULA 4)	ROOM B (AULA 5)	ROOM C (AULA 7)	ROOM D (AULA 8)	ROOM E (SALÓN DE ACTOS)
11.40-12.00	**IL31.** *Josef Paldus*. Coupled-Cluster Approaches to Excited States	**IL32**. *Henrik Kjaergaard* Spectroscopy of binary molecular complexes	**IL33**. *Javier Fdez Sanz* Mechanism of the Water-Gas Shift Reaction: Insights from First Principles Calculations	**IL35**. *Adrian Mulholland* Enzyme dynamics, conformations and catalysis	**IL34**. *Benedito J.C. Cabral* Electronic properties of hydrogen bond networks: a theoretical approach based on sequential statistical mechanics/ quantum mechanical calculations
12.00-12.20	**IL36.** *Cristof Hättig* Accurate and efficient approximations to explicitly correlated coupled-cluster singles and doubles, CCSD-F12	**IL37**. *Marie-Pierre Gaigeot* Anharmonic vibrational spectroscopy with DFT-MD simulations	**IL38**. *David Loffreda* Solvation of Organic Molecules at Liquid/ Metal Interfaces from First-Principles Simulations	**IL40**. *Iñaki Tuñón* Unraveling evolution through molecular simulations. Catalysis in the alkaline phosphatase superfamily	**IL39**. *Per Ake Malmqvist* Hydrogen bonds to proton transfer chains in water
12.20-12.40	**IL41.** *Shuhua Li. A* New Coupled Cluster Method for Bond-breaking Potential Energy Surfaces	**IL42**. *Michael Filatov* Understanding the dynamics behind the photoisomerization of light-driven molecular rotary motors	**IL43**. *Hirofumi Sato* Impact of solvation: efficient models for chemical reaction and equilibrium in solution phase	**IL45.** *Leif Eriksson* Active state dynamics and catalytic mechanism of sortase A enzymes	**IL44**. *Theresa Windus* Environmental chemistry with a high performance kick

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12.40-12.50	**OC6.** *Andreas Köhn* Multi-Reference Coupled-Cluster: The Internally Contracted Approach	**OC7**. *Carine Clavaguera* Estructure and IR spectrum of the gramicidin S peptide as a β-Sheet Model	**OC8**. *Albert Bruix* Study of the interaction of Pt_x species with oxidized and reduced CeO_2 (111)	**OC10**. *Silvia Ferrer* Molecular simulations of promiscuous activities: the Mbtl case	**OC9**. *Angelika Baranowska* Importance of electron correlation effects and basis set superposition error in calculations of interaction energies and interaction induced electric properties in hydrogen-bonded complexes. A model study
12.50-13.00	**OC11.** *Francesco A. Evangelista* An Orbital-Invariant Internally Contracted Multireference Coupled Cluster Approach	**OC12**. *Gregory S. Tschumper* Effects of dihydrogen bonding on the structure, energetics and vibrational spectrum of BH_3NH_3	**OC13**. *Antonio Márquez* Understanding acetaldehyde thermal chemistry on the TiO_2 (110) rutile surface: from adsorption to reactivity	**OC15**. *Michael Shokhen* Rationalization of the driving force controlling pk_a of catalytic residues and enzyme acid/base catalysis	**OC14**. *Ekaterina Izgorodina* Nature of hydrogen bonding in charged complexes and ionic liquids
13.00-15.30	LUNCH BREAK				

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15.30-17.30	**M3.5** Computational Strategies for biomolecular systems. (Chair: *Javier Luque*)	**M3.2** Quantum Montecarlo (Chair: *Bruce Garrett*)	**M3.3** Clusters/ nanostructures I (Chair: *Minh To Nguyen*)	**M3.4** Inorganic photochemistry/ Transition metals (Chair: *Timofei Privalov*)	**M3.1** DFT: New developments/ applications I (Chair: *Clemence Corminboeuf*)
15.30-15.50	**IL50.** *Maria J. Ramos* Computational proteomics	**IL47**. *Ali Alavi* Quantum Monte Carlo approach to the Full CI problem	**IL48**. *Joachim Sauer* Occupation of Ce-f states in defective CeO_2 and mixed CeO_2/VO_2 gas phase clusters DFT compared to experiment	**IL49**. *Josef Michl* Exciton Relaxation in Saturated Systems: Peralkylated Oligosilanes	**IL46**. *Gustavo Scuseria* Strong Correlations from Constrained Mean-Field Approaches
15.50-16.10	**IL55.** *Modesto Orozco* The travel of a computational chemistry along DNA	**IL52**. *Michel Caffarel* Recent advances in computing forces with quantum Monte Carlo	**IL53**. *Andrés Reyes* A theoretical study of the quantum state of atoms trapped inside fullerenes	**IL54**. *Chantal Daniel* Spin-orbit effects on the photophysics and photochemistry of rhenium (I) complexes	**IL51**. *Lucas Visscher* WFT-in-DFT methods for excited states
16.10-16.30	**IL60.** *Ulf Ryde* Tests and improvements of end-point methods for ligand-binding affinities	**IL57**. *Alejandro Ramírez-Solís* Benchmarking DFT spin densities with Quantum Monte Carlo. The $CuCl_4$ case: correct UKS transition energies but wrong DFT spin-densities	**IL58**. *Shridhar R. Gadre* Electrostatics- and MTA-enabled Molecular Cluster Assembler	**IL59**. *Coen De Graaf* Light-induced magnetism in copper octacyanomolybdates	**IL56**. *Tom Ziegler* The Description of Excited States by Constricted Variational Density Functional Theory

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16.30-16.50	**IL65.** *H. Bernhard Schlegel* Exploring Potential Energy Surfaces for Enzymatic Reactions Using QM/MM Calculations	**IL62**. *Arne Lüchow* Single electron densities: a new tool to analyse and visualize molecular wave functions using Quantum Monte Carlo	**IL63**. *Ilya G. Kaplan* Why metal atoms with closed valence shell form chemically bonded clusters A_n (n > 2): alkaline-earth clusters	**IL64**. *Denis Jacquemin* TD-DFT simulations of coupled photochromes	**IL61**. *Stefan Grimme* Effect of London Dispersion Energy on the Thermochemical Properties of Molecules
16.50-17.10	**IL70.** *Kevin J. Naidoo* Resolving the Historical Competition between Sampling and Levels of QM Theory in QM/MM Simulations of Reactions	**IL67**. *William A. Lester* Quantum Monte Carlo for the Electronic Structure of Molecular Systems	**IL68**. *Gianfranco Pacchioni* Oxides at the nanoscale: new structures, new functions, and new materials	**IL69**. *Ria Broer* Transitions in transition metal compounds	**IL66**. *Alexandre Tkatchenko* Van der Waals Interactions in Molecules and Solids: Self-Consistent Screening and Many-Body Effects
17.10-17.20	**OC20**. *Marwa Farag* Vibrational energy relaxation of small peptides in solution: the effect of polarization and charge transfer	**OC17**. *Justin Elenewski* Path Integral Monte Carlo Simulations of Proton Tunneling In Effective Ab Initio Potential Landscapes	**OC18**. *Itamar Borges* How to Find an Optimum Cluster Size through Topological Site Properties: MoS_x Model Clusters	**OC19**. *Sebastian Kozuch* What makes for a good catalytic cycle? Insights from the energetic span model	**OC16**. *Geroge A. Petersson* A Density Functional with Spherical Atom Dispersion Terms

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17.20-17.30	**OC25**. *Pedro A. Fernandes* Methodologic issues that determine the accuracy of the computational prediction of enzymatic mechanisms	**OC22**. *Basile F.E. Curchod* Trajectory-based solution of the nonadiabatic quantum dynamics equations: an on-the-fly approach for molecular dynamics simulations	**OC23**. *Massimiliano Bartolomei* Theoretical studies for the oxygen tetramer: intermolecular bonding and implications for the ε solid phase	**OC24**. *Elke Pahl* Toward the melting of mercury: A challenge to computational chemistry	**OC21**. *Alisa Krishtal* Modeling of dispersion interactions in DFT
17.30-18.00	COFFEE BREAK				
18.00-19.30	**M4.5** Adsorption/ Surface interactions (Chair: *Lorenzo Maschio*)	**M4.2** Chirality (Chair: Robert Berger)	**M4.3** Astrochemistry/ Chemistry of the atmospheres. I (Chair: *Josep M. Anglada*)	**M4.4** Biomolecular Interactions (Chair: *Pedro B. Coto*)	**M4.1** Solvation (Chair: *Kaline Coutinho*)
18.00-18.20	**IL75**. *Stephan Irle* Quantum chemical molecular dynamics simulations of graphene hydrogenation	**IL72**. *Ibon Alkorta* Chiral discrimination in complexes of molecules of biological interest	**IL73**. *Joe Francisco* New Insight into HOCO Radical Chemistry	**IL74**. *Russell J. Boyd* Electronic Energy Changes Associated with Guanine Quadruplex Formation	**IL71**. *Manuel Ruiz-Lopez* Simulation of Chemical Reactions at Water/ Hydrophobic Interfaces

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18.20-18.40	**IL80**. *Laura Gagliardi* The development of first-principle force fields for modeling the adsorption of CO_2 in metal-organic frameworks	**IL77**. *Peter Schwerdtfeger* Towards the first measurement of parity violation in chiral molecules: New attempts and future prospective	**IL78**. *Tore Brinck* Theoretical and experimental characterization of new nitrogen oxides: the case of trinitramide	**IL79**. *Matthias Bickelhaupt* Covalency in hydrogen bonds causes cooperativity in guanine quartets	**IL76**. *Ian Williams* Ensemble-Averaged QM/MM Kinetic Isotope Effects for Condensed-Phase SN2 Reations
18.40-19.00	**IL85**. *Diego Troya* Theoretical studies of reactions between gases and organic surfaces	**IL82**. *Antonio Rizzo* Nonlinear spectroscopies and chirality	**IL83**. *Ivan Cernusak* Atmospheric chemistry of iodine **M4.3.1** More on excited states & spectroscopy	**IL84**. *Stacey Wetmore* Accurate Modeling of DNA-Protein Interactions and DNA Repair Processes	**IL81**. *Raghavan Sunoj* Microsolvated Transition State Models for Improved Insights on Mechanism and Stereoselectivity in Organic Reactions
19.00-19.10	**OC30**. *M. Verónica. Ganduglia-Pirovano* Application of hybrid exchange-correlation functionals to reduced ceria	**OC27**. *Oliver Weingart* Chiral pathways and periodic decay in cisazobenz ene photodynamics	**OC28**. *Miroslav Urban* Theoretical study on properties of the valence excited states of acetone	**OC29**. *Juan M. Ortiz-Sánchez* Structure based discovery of novel druggable pockets on rho family GTPases	**OC26**. *Junming Ho* Predicting pk_a: theory and applications

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MONDAY JULY 18 FACULTY OF MEDICINE

	ROOM A (AULA 4)	ROOM B (AULA 5)	ROOM C (AULA 7)	ROOM D (AULA 8)	ROOM E (SALÓN DE ACTOS)
19.10-19.20	**OC35**. *Kari Laasonen* Study of some reaction on the surface of a nanosize iron cluster	**OC32**. *Jonathan Hirst* Computing the chiral two-dimensional UV spectroscopy of proteins	**OC33**. *Ralf Tonner* Vibrational properties of organic thin films from theory and experiment	**OC34**. *Carolina Estarellas* Anion-π interactions in real life.	**OC31**. *Niels Drechsel* Analytical Non-Polar Solvation Free Energy for the Sea-Water Model
19.20-19.30	**OC40**. *Christophe Mager-Maury* Hydrogen induced Reconstruction for Supported Pt Clusters: Metal-support Interaction versus Surface-Hydride	**OC37**. *José I. García* Surface confinements effects in enantioselective catalysis: ligand desing and computational studies	**OC38**. *Malgorzata Biczysko* Toward an understanding of chlorophylls: simulation of the coordination and vibrational effects in the uv-vis spectra	**OC39**. *Wenning Wang* Conformational Dynamics and Translocation Mechanism of ABC Transporters	**OC36**. *Andriy Kovalenko* SCF coupling of KS-DFT and OFE-DFT with statistical-mechanical 3D-RISM-KH molecular theory of solvation for multiscale treatment of nanochemistry and photochemistry in solution
19.30-19.40	**OC45**. *Angeles Pulido* Theoretical investigation of gold nanoparticles supported on graphene sheets	**OC42**. *Walter Fabian* Axially chiral bisquinolones as fluorophores	**OC43**. *Anthony D. Dutoi* Time-resolved pump-probe spectroscopy to follow valence electron motion	**OC44**. *Petra Imhof* The role of metal ions in DNA cleavage	**OC41**. *Regla Ayala* Polonium solution chemistry: new insights into the physicochemical behaviour of Po(IV) in water

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TUESDAY JULY 19

9.00-11.00	**TU.1 Plenary Session (Chair: Enrico Clementi)** **AUDITORIO DE GALICIA**
9.00-9.40	**PL4. Evert Jan Baerends.** Beyond DFT
9.40-10.20	**PL5. Jeremy Harvey.** Computational insight into catalysis: mechanism, selectivity and kinetics
10.20-11.00	**PL6. Leticia González.** Shedding light on functional molecules
11.00-11.30	**COFFEE BREAK**
11.30-13.30	**Poster Session II** (PII-1 to PII-299) **FACULTY OF ECONOMY**
13.30-15.30	**LUNCH BREAK**
16.00	**EXCURSION**

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WEDNESDAY JULY 20 FACULTY OF MEDICINE

	ROOM A (AULA 4)	ROOM B (AULA 5)	ROOM C (AULA 7)	ROOM D (AULA 8)	ROOM E (SALÓN DE ACTOS)
9.00-10.30	**W1.1** Aromaticity (Chair: *Shogo Sakai*)	**W1.5** Non-covalent interactions (Chair: *Takeshi Sato*)	**W1.3** Reaction Mechanisms (Chair: *Devesh Kumar*)	**W1.4** Bond activation reactions (Chair: *Gilles Ohanessian*)	**W1.2** Methodology developments/ large molecules (Chair: *Jan Řezáč*)
9.00-9.20	**IL86.** *Alexander I. Boldyrev* Deciphering delocalized bonding in chemical species	**IL90**. *Sotiris Xantheas* Guest-host interactions in hydrate lattices and functional molecules	**IL88**. *James T. Hynes* On the Mechanism of Water Oxidation by the Blue Dimer	**IL89**. *Helmut Schwarz* Homolytic C-H Bond Activation: The Role of Oxygen-Centered Radicals and Mechanistic Aspects	**IL87**. *Krishnan Ragavachari* Towards Accurate Electronic Structure Methods for Large Molecules
9.20-9.40	**IL91**. *Miquel Solà* Recent advances in the aromaticity of inorganic clusters and fullerenes	**IL95**. *G. Narahari Sastry* Range and relevance of cation-aromatic interactions in macromolecular assemblies	**IL93**. *Henry S. Rzepa* Mechanistic explorations of reactions involving ion-pairs	**IL94**. *Yitzhak Apeloig* Recent Theoretical Studies of Low-Coordination Silicon Compounds	**IL92**. *Hans-Joachim Werner* Explicitly correlated local coupled cluster methods for large molecules
9.40-10.00	**IL96**. *Marcin Palusiak* The new aromaticity measure based on one-electron density function	**IL100**. *Miklos Kertesz* Short contacts between π-stacking neutral organic radicals	**IL98**. *Elfi Kraka* From reaction path curvature to reaction phases and reaction mechanism	**IL99**. *Alejandro Toro-Labbé* On the Physical Nature of Activation Processes	**IL97**. *Piotr Piecuch* Local coupled-cluster methods for chemical reaction pathways involving large molecular systems and their multi-level generalizations

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WEDNESDAY JULY 20 FACULTY OF MEDICINE

	ROOM A (AULA 4)	ROOM B (AULA 5)	ROOM C (AULA 7)	ROOM D (AULA 8)	ROOM E (SALÓN DE ACTOS)
10.00-10.20	**IL101**. *Pratim K. Chattaraj* All-metal aromaticity and conceptual DFT	**IL105**. *Tim Clark* Hydrogen- and Halogen-Bonds: A Grand Oversimplified Theory of σ-Holes	**IL103**. *Jörn. Manz* Panta Rhei – electron fluxes during chemical reactions	**IL104**. *Shigeyoshi Sakaki* Heterolytic C-H σ-Bond Activation Reaction: Driving Force, Regioselectivity, Orbital Mixing, and Its Application to Pd-Catalyzed Direct Cross-Coupling Reaction	**IL102**. *Frank Neese* Recent developments in single correlation methods for large molecules
10.20-10.30	**OC46**. *Israel Fernandez* Double Group Transfer Reactions: Aromaticity and Activation Strain	**OC50**. *Anna K. Croft* Towards an understanding of organic processes in ionic liquids	**OC48**. *Carol Parish* Decomposition mechanisms of thiophene	**OC49**. *Laimutis Bytautas* New ab initio approaches for accurate description of the bond breaking: How close are we to the "spectroscopic accuracy"?	**OC47**. *Jan Řezáč* S66: new dataset of benchmark interaction energies
10.30-11.00	COFFEE BREAK				

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WEDNESDAY JULY 20 FACULTY OF MEDICINE

	ROOM A (AULA 4)	ROOM B (AULA 5)	ROOM C (AULA 7)	ROOM D (AULA 8)	ROOM E (SALÓN DE ACTOS)
11.00-13.00	**W2.5** Electronic spectra/one & two photon excitations. Symposium in memoriam of Luis Serrano Andrés (Chair: *Lluis Blancafort*)	**W2.2** Explicitly correlated methods/ Choleski decomposition (Chair: *Sergei Gusarov*)	**W2.3** Functional materials (Chair: *Carmen J. Calzado*)	**W2.4** Porous materials/ gas storage (Chair: *Andriy Kovalenko*)	**W2.1** DFT: New developments/ applications II (Chair: *Suehiro Iwata*)
11.00-11.20	**IL110**. *Anna Krylov* Non-Condon effects in one- and two-photon absorption spectra of the green fluorescent protein	**IL107**. *Willem Klopper* Interference-corrected explicitly-correlated second-order perturbation theory	**IL108**. *Enrique Ortí* Electroluminescence from ionic transition-metal complexes	**IL109**. *Richard Catlow* Computer Modelling of Microporous and Oxide Catalysts	**IL106**. *Axel Becke* A density-functional model of strong correlation
11.20-11.40	**IL115**. *Attila Császár* Spectroscopic Networks	**IL112**. *David Sherrill* Extending the Reach of Symmetry-Adapted Perturbation Theory Through Density Fitting and Natural Orbitals	**IL113**. *Ji Hoon Shim* Density functional calculations of the hydrocarbon K_3picene superconductor near the metal-insulator transition	**IL114**. *Aatto Laaksonen* Computer modelling and simulations of carbon capture and separation in porous materials	**IL111**. *Martin Kaupp* Improved Local Hybrid Functionals

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WEDNESDAY JULY 20 FACULTY OF MEDICINE

	ROOM A (AULA 4)	ROOM B (AULA 5)	ROOM C (AULA 7)	ROOM D (AULA 8)	ROOM E (SALÓN DE ACTOS)
11.40-12.00	**IL120**. *Benedetta Mennucci* Modeling environment effects on fluorescence with hybrid quantum mechanical/classical approaches	**IL117**. *Roland Lindh* Cholesky decomposition casscf gradients	**IL118**. *Marta B. Ferraro* Modified genetic algorithm for crystal structure prediction	**IL119**. *Claudio Zicovich-Wilson* Can the presence of occluded species revert the stability of two molecular sieves? The cases of silica Theta-1 and ITQ-12	**IL116**. *Hannes Jónsson* Orbital density dependent energy functionals: implementation and application to atoms & oxides
12.00-12.20	**IL125**. *Vladimiro Mujica* The role of photo-excited states of molecule-semiconductor nanoparticles hybrids in nanosensors, solar cells and photo-catalysis	**IL122**. *Edward Valeev* Quantum Chemistry Beyond Atomic Orbitals and Slater Determinants	**IL123**. *Jin Yong Lee* Magnetization control of silicon carbon nanoribbons: First principle calculations	**IL124**. *Jürgen Eckert* Rotational transitions and potential energy surfaces for hydrogen adsorbed in metal organic frameworks	**IL121**. *Paul Geerlings* Methodological advances in conceptual DFT
12.20-12.40	**IL130**. *Mar Reguero* Intramolecular charge transfer in aminopyrimidines. Different fluorescent behaviour observed in different derivatives explained by a computational study	**IL127**. *Jozef Noga* Alternative orbital optimization scheme based on non-unitary transformation	**IL128**. *Kim Baldridge* Structure and materials properties of corannulene derivatives on metallic surfaces and in the crystalline bulk	**IL129**. *Richard Wong* Mechanism of dehydrogenation in chemical hydrogen storage materials	**IL126**. *Hiromi Nakai* Novel approaches in density functional theory to treat core excitations and weak interactions

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WEDNESDAY JULY 20 FACULTY OF MEDICINE

	ROOM A (AULA 4)	ROOM B (AULA 5)	ROOM C (AULA 7)	ROOM D (AULA 8)	ROOM E (SALÓN DE ACTOS)
12.40-12.50	**OC55**. *Quansong Li* Potential energy surface for the photophysics of adenine-uracil monophospate dimer	**OC52**. *Toru Shiozaki* Multi-reference Explicitly Correlated F12 Theories	**OC53**. *Antti J. Karttunen* Mechanical properties of semiconducting group 14 clathrate frameworks	**OC54**. *Michele Pavone* First-principles modeling of perovskite type transition metal oxides as cathode materials for solid oxide fuel cell applications	**OC51**. *Yves A. Bernard* Noncollinear spin-flip time-dependent density function theory: a benchmark study
12.50-13.00	**OC60**. *Israel González-Ramírez* CASPT2 Investigation on the N1-H and N3-H Bond Dissociation by Low Energy Electrons in Uracil	**OC57**. *Clemence Corminboeuf* Direct Assessment of Pi-Conjugation Effects on Molecular Properties	**OC58**. *Marek Sierka* Combining theory and experiment in structure resolution of low-dimensional materials	**OC59**. *Jeroen Van der Mynsbrugge* Investigation of confinement effects on zeolite-catalyzed methylation reactions	**OC56**. *Felix Kannemann* Van der Waals interactions in density-functional theory: basis sets
13.00-15.30	LUNCH BREAK				

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	ROOM A (AULA 4)	ROOM B (AULA 5)	ROOM C (AULA 7)	ROOM D (AULA 8)	ROOM E (SALÓN DE ACTOS)
15.30-17.30	**W3.1** Theory II (Chair: *Gregory S. Tschumper*)	**W3.2** Photodynamic simulations (Chair: *Mario Barbatti*)	**W3.3** VB theory (Chair: *David Danovich*)	**W3.4** Clusters/ Nanostructures II (Chair: *Rafael Escribano*)	**W3.5** Organic reaction mechanisms (Chair: *Evgenyi Gromov*)
15.30-15.50	**IL131**. *Vidar. R. Jensen* An evolutionary algorithm method for de novo optimization of functional coordination compounds	**IL132**. *Hans Lischka* Simulation of Defect Transport in Stacked π-Systems	**IL133**. *Jeppe Olsen* Wave function methods for complexes with three or more transition metal atoms	**IL134**. *Athanassios Tsipis* Aromatic $[c\text{-}M_3(\mu_2\text{-}X_3]n(C_6H_6)_m$ (M = coinage metal atom; X = halogen atom; n, m ≤ 2) superclusters	**IL135**. *Keiji Morokuma* Computational Studies of Chemical Reactions of Molecular Systems: Overview of Our Recent Activities
15.50-16.10	**IL136**. *Ivano Tavernelli* Nonadiabatic molecular dynamics with explicit external electrostatic and electromagnetic fields	**IL137**. *Horst Köppel* Ab initio quantum dynamical treatment of elementarynonadiabatic photoreactions	**IL138**. *Yirong Mo* Probing the intra- and inter-molecular interactions	**IL139**. *Arnout Ceulemans* The boron conundrum	**IL140**. *Nela Mora-Diez* Nucleophilic Additions to Carbonyl Groups Via Specific Acid Catalysis Mechanism: Rule or Exception?
16.10-16.30	**IL141**. *Johannes Kästner* Accurate tunneling rates in large systems: implications for biochemical reactions	**IL142**. *Marco Garavelli* Conical intersection dynamics in the rhodopsin and isorhodopsin primary event	**IL143**. *Wei Wu* Ab initio Valence Bond Methods for Dynamic Correlation: VBPT2 and DFVB	**IL144**. *Carles Bo* Challenges in polyoxometalates chemistry: what's inside those molecular oxide nanocapsules?	**IL145**. *Athanassios Nicolaides* Isomerizations of dimers of highly pyramidalized alkenes

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	ROOM A (AULA 4)	ROOM B (AULA 5)	ROOM C (AULA 7)	ROOM D (AULA 8)	ROOM E (SALÓN DE ACTOS)
16.30-16.50	**IL146**. *Alberto Vela* The density gradient analysis: a new tool to study chemical interactions	**IL147**. *Mirjana Eckert-Maksic* Formamide as the model compound for photodissociation of the peptide bond	**IL148**. *Chaer Nascimento* Quantum interference and the chemical bond	**IL149**. *Eluvathingal D. Jemmis* Ten years of mno rule in boron chemistry	**IL150**. *Max Holthausen* The base-induced disproportionation of perchlorosilanes - a mechanistic scenario
16.50-17.10	**IL151**. *Jan M. Martin* What can we learn about dispersion from the conformer surface of small alkanes?	**IL152**. *Benoît Champagne* A vibronic approach for simulating and interpreting resonant Raman spectra of organic molecules	**IL153**. *Benoît Braïda* A Valence Bond view of hypervalency: the XeF_2 case	**IL154**. *Gabriel Merino* Fluxional boron clusters	**IL155**. *Peter R. Schreiner* Tunneling Control of Chemical Reactions
17.10-17.20	**OC61**. *Meredith J.T. Jordan* A phase space theory for roaming reactions	**OC62**. *Inés Corral* Kasha or non-kasha? A mechanistic and dynamical insight into the intramolecular hydrogen transfer reaction in o-nitrobenzaldehyde	**OC63**. *Peifeng Su* VB-EFP: A new QM/MM scheme based ab inito valence bond theory	**OC64**. *Josep M. Oliva* Electronic structure in icosahedral heteroborane chemistry	**OC65**. *Michael B. Hall* Mechanism of the reaction of nickel bis(dithiolenes) with alkenes

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	ROOM A (AULA 4)	ROOM B (AULA 5)	ROOM C (AULA 7)	ROOM D (AULA 8)	ROOM E (SALÓN DE ACTOS)
17.20-17.30	**OC66**. *Tomoko Akama* Real-time TDHF/ TDDFT calculations for electron dynamics	**OC67**. *Jesús González-Vázquez* Mixed quantum-classical dynamics under strong fields: a numerical tool to follow quantum adiabatic dynamics in full dimension	**OC68**. *Dan T. Major* Nuclear quantum effects in enzyme catalysis – from development to application	**OC69**. *Francesca Spyrakis* The hydrophobic "breathing" of cytoglobin	**OC70**. *Dmitry Nerukh* Disecting peptide conformational transitions: unique water dynamics
17.30-18.00	COFFEE BREAK				
18.00-19.40	**W4.1** Relativistic effects. II (Chair: *Robert Ponec*)	**W4.2** Quantum Chemical topology (Chair: *Peeter Burk*)	**W4.3** Correlation & molecular properties/ dispersion (Chair: *Rosa Caballol*)	**W4.5** Astrochemistry/ Chemistry of the atmospheres. II (Chair: *Marzio Rosi*)	**W4.4** Biomolecular Interactions/ Proton and electron transfer. Symposium in Memoriam of Zvonko Maksic (Chair: *David Smith*)
18.00-18.20	**IL156**. *Pekka Pyykkö* Recent results in relativistic quantum chemistry: from the lead battery to the periodic system	**IL157**. *Angel Martín Pendás* Some recent developments in quantum chemical topology	**IL158**. *Tatiana Korona* First- and second-order molecular properties from expectation-value coupled cluster theory	**IL160**. *Jean-Claude Rayez* Some theoretical contributions in heterogeneous chemistry	**IL159**. *Luis G. Arnaut* Proton-coupled electron transfer: the connection between (adiabatic) proton and (nonadiabatic) electron transfer theories

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	ROOM A (AULA 4)	ROOM B (AULA 5)	ROOM C (AULA 7)	ROOM D (AULA 8)	ROOM E (SALÓN DE ACTOS)
18.20-18.40	**IL161**. *Xiaoyan Cao* Relativistic Energy-consistent Ab Initio Pseudopotentials And Their Application to the Study of the Separation of Am(III)/Cm(III) from Eu(III) with Cyanex 301	**IL162**. *Paul L. A. Popelier* Intramolecular Polarisation by Machine Learning	**IL163**. *Trygve Helgaker* Molecules in strong magnetic fields	**IL165**. *Einar Uggerud* The formose reaction and interstellar carbohydrate formation	**IL164**. *Janez Mavri* Molecular Simulation of Proton Transfer in Biological Systems
18.40-19.00	**IL166**. *Bogumil Jeziorski* QED effects in molecular spectra and structure	**IL167**. *Andreas Savin* Chemical bonds from quantum mechanical probabilities	**IL168.** *Paul Ayers* Can One Oxidize an Atom by Reducing the Molecule that Contains it?	**IL170**. *Antonio Largo* Computational Astrochemistry: Ion-Molecule Processes in the Synthesis of Interstellar Glycine	**IL169**. *H. Nakatsuji* Helical Structure and Circular Dichroism Spectra of DNA: SAC-CI Study
	W4.1.1 More on catalysis	**W4.2.1** Reactivity		**W4.5.1** More on solvation	
19.00-19.10	**OC71**. *Albeiro Restrepo* Spin-Orbit Effects in Molecular Geometries	**OC72**. *Vincent Tognetti (1286)* On the use of Bader's atoms in molecules theory for the study of agostic bonds	**OC73**. *Alessandro Erba* An MP2 study of pressure-induced phase transitions in solid nitrogen: the role of dispersive interactions	**OC75**. *Petr Slavicek* What can theoretical chemistry tell us on solvated electron: from water photochemistry to biophysics	**OC74**. *John C. Hackett* Coupled Electron Transfer and Proton Hopping in P450-Catalyzed Androgen Aromatization

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	ROOM A (AULA 4)	ROOM B (AULA 5)	ROOM C (AULA 7)	ROOM D (AULA 8)	ROOM E (SALÓN DE ACTOS)
19.10-19.20	**OC76**. *Zhipan Liu* First-principles simulation of electrocatalytic reactions	**OC77**. *François Zielinski* Condensed atomic descriptors for reactivity: a comparative study	**OC78**. *Javier Carrasco* To wet or not to wet? Dispersion forces tip the balance for water ice on metals	**OC80**. *Zexing Cao* Hydration of Carbonyl Groups: Insight into the Concerted and Stepwise Mechanism Argument from Ab Initio Calculations	**OC79**. *Robert Vianello* Hydrogen bond dynamics and computational vibrational spectroscopy in aqueous solution: the case study of histamine monocation
19.20-19.30	**OC81**. *Andrei L. Tchougréeff* Catalytic action of transition metal porphyrins in quadricyclane to norbornadiene isomerization. Quantum mechanical análisis	**OC82**. *András Stirling* H_2CO_3 forms via HCO_3- in water	**OC83**. *Takeshi Sato* Density-dependent dispersion interaction from local response approximation	**OC85**. *Li Xiang-Yuan* A Modification to Marcus Theory: Novel Expression of Solvent Reorganization Energy by Constrained Equilibrium Principle	**OC84**. *Fatima Chami* Structure and organisation in chromonic systems
19.30-19.40	**OC86**. *Tomifei Privalov* Mechanistic aspects of donor-acceptor catalysis of atom-transfer processes	**OC87**. *Laurent Cantrel* Ability of theoretical chemistry to predict thermochemistry and reactivity of gaseous caesium species of nuclear safety interest	**OC88**. *Stephan N. Steinmann* A Generalized-Gradient Approximation Exchange Hole Model for Dispersion Coefficients	**OC90**. *G. Scalmani* The best kept secret in reaction field theory	**OC89**. *Jean-Yves Salpin* Interactions of cisplatin with nucleotides: a combined experimental and theoretical study
21.30	**CONCERT AT THE CATHEDRAL**				

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9.00-11.00	**TH1.5** Metalloproteins/ Alzheimer dissease (Chair: *Valérie Brenner*)	**TH1.2** Force fields/ Free energy landscapes (Chair: *Jiali Gao*)	**TH1.3** Molecular devices/self assembling (Chair: *Christian van Alsenoy*)	**TH1.4** Excited states in biomolecules (Chair: *Adelia Aquino*)	**TH1.1** Electron correlation theory / linear scaling (Chair: *Anthony D. Dutoi*)
9.00-9.20	**IL175**. *Arvi Rauk* Peptide-Peptide Interactions by MD-AFM: Anti-aggregation Agents and the Amyloid Beta Peptide of Alzheimer Disease	**IL172**. *Wilfred van Gunsteren* Methodological advances in the computation of relative free energies	**IL173**. *Tamar Seideman* Current control in the Nanoscale	**IL174**. *Walter Thiel* QM/MM Studies of Enzymes and Excited States	**IL171**. *Markus Reiher* New Electron Correlation Theories for Transition Metal Compounds
9.20-9.40	**IL180**. *Mariona Sodupe* Three dimensional models of Cu_2+-Aβ(1-16) complexes from computational approaches	**IL177**. *Allan. E. Mark* Improving the structures of ligand molecules in X-ray complexes: An Automated force field Topology Builder (ATB) and repository for drug-like molecules	**IL178**. *Manuel Alcamí* Self-assembly of electron-donor/ acceptor molecules on metal surfaces	**IL179**. *Peter Szalay* Coupled cluster theory with triples on biosystems? Study of the excited states of nucleobases and nucleosides	**IL176**. *Angela Wilson* Accurate energetics for ground and excited states across the periodic Table: the single and multireference composite approaches CCAA and MR-CCCA

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9.40-10.00	**IL185**. *Carmay Lim* Competition Between Li^{+} and Mg^{2+} in Metalloproteins. Implications for Lithium Therapy	**IL182**. *Masataka Nagaoka* Free energy landscape of glycine isomerization in aqueous solution: application of ab initio QM/MM MD-free energy gradient (FEG) method	**IL183**. *Kwang S. Kim* Ultrafast DNA Sequencing and Nano-optics/photonics	**IL184**. *Johannes Neugebauer* First-principles calculation of the absorption spectrum of light-harvesting complex II	**IL181**. *Mark Hoffmann* Nonadiabatic coupling terms for generalized van Vleck multireference perturbation theory
10.00-10.20	**IL190**. *Avital Shurki* Copper Chaperones – Copper(I) Keepers	**IL187**. *Yun-Dong Wu* Force Field Development based on Amino Acid Rotamer Distributions	**IL188**. *Jorge M. Seminario* Moletronics for the post CMOS era	**IL189**. *Silvio Canuto* The absorption spectrum of chlorophyll c in methanol. A sequential QM/MM study	**IL186**. *Christian Ochsenfeld* Linear- and Sub-Linear Scaling Quantum-Chemical Methods
10.20-10.40	**IL195**. *Xabi López* Aluminium in biological systems	**IL192**. *Jan Halborg Jensen* Blurring the boundary between linear scaling QM, QM/MM and polarizable force fields	**IL193**. *Piero Ugliengo* Molecular Recognition at the Surfaces of Hydroxyapatite Modeled by Periodic DFT Methods Based on Localized Orbitals	**IL194**. *Lyudmila V. Slipchenko* Effective fragment potential method: applications to electronic spectroscopy in solvents and proteins	**IL191**. *Thomas B. Pedersen* Linear scaling local density fitting based on Cholesky decompositons

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	ROOM A (AULA 4)	ROOM B (AULA 5)	ROOM C (AULA 7)	ROOM D (AULA 8)	ROOM E (SALÓN DE ACTOS)
10.40-10.50	**OC95**. *Sabyashachi Mishra* Role of β-secretase in Alzheimer's disease: a computational approach	**OC92**. *Davide Branduardi* Free energy calculations of enzymatic reactions with path collective variables	**OC93**. *Tell Tuttle* Virtual Screening for Peptide Self-Assembly	**OC94**. *Dana Nachtigallová* Photodynamics of 4-aminopyrimidine embedded within single and double strands of nucleic acids	**OC91**. *Jesse. J. Lutz* Performance of completely renormalized equation-of-motion coupled-cluster methods on excited-state potential energy curves for the dissociation of water
10.50-11.00	**OC100**. *Ran Friedman* Metal ions in life: ions at the protein surface	**OC97**. *Luigi Gervasio* Understanding the plasticity of c-Src tyrosine kinase through very long molecular dynamics simulations and experimentally-validated free energy calculations	**OC98**. *Alister J. Page* Understanding Nanoscale Self-Assembly Processes Using QM/MD: Mechanisms of Carbon Nanotube Nucleation and Growth	**OC99**. *Feng Wang* Novel combination of spectroscopic simulation and synchrotron sourced spectroscopy to study biomolecules	**OC96**. *Sonia Coriani* Coupled cluster study of near-edge X-ray absorption spectra

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	ROOM A (AULA 4)	ROOM B (AULA 5)	ROOM C (AULA 7)	ROOM D (AULA 8)	ROOM E (SALÓN DE ACTOS)
11.00-11.10	**OC105**. *Sanja Tomić* Step Forward in Understanding Mechanism of Non-heme Fe^{2+} Dependent Dioxyhenase Dke1 Catalysis	**OC102**. *Michal Kolář* Treatment of the halogen bond with a current biomolecular empirical force field	**OC103**. *José M. Hermida-Ramón* Analysis of the SERS spectrum of several substances by using theoretical methodology. Evaluating a dipole coupling model and a detuning of the excitation frequency model	**OC104**. *Nicolas Onofrio* Analysis of the singlet-triplet splitting computed by the DFT-broken symmetry method: is J_{BS} an exchange coupling constant?	**OC101**. *Nicola Gaston* Incremental coupled-cluster calculations for zinc clusters; how to close the gap between small clusters and the bulk metal
11.10-11.40	COFFEE BREAK				
12.00	BOTAFUMEIRO EXHIBITION AT THE CATHEDRAL				
13.00-15.30	LUNCH BREAK				

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THURSDAY JULY 21 FACULTY OF MEDICINE

	ROOM A (AULA 4)	ROOM B (AULA 5)	ROOM C (AULA 7)	ROOM D (AULA 8)	ROOM E (SALÓN DE ACTOS)
15.30-17.10	**TH2.1** GPU Technology (Chair: *Jiří Pittner*)	**TH2.2** Chemical dynamics/ reaction pathways (Chair: *Antonio Laganà*)	**TH2.3** Nanostructures (Chair: *Fernando Martín*)	**TH2.4** Organometallic chemistry/homogeneous catalysis (Chair: *Agustí Lledós*)	**TH2.5** Cycloadditions (Chair: *Angels González Lafont*)
15.30-15.50	**IL196**. *Mark Gordon* Quantum chemistry on graphical processing units: it ain't all a bed of roses	**IL197**. *Bill Hase* Chemical Dynamics Simulations of Gas-Phase $X^- + CH_3Y \rightarrow XCH_3 + Y^-$ SN2 Nucleophilic Substitution Reactions	**IL198**. *Stefano Evangelisti* Finite-size effects in graphene nanostructures	**IL199**. *Brian Yates* Understanding organometallic chemistry: high-oxidation state palladium systems	**IL200**. *Kendall N. Houk* Dynamics and mechanisms of cycloadditions
15.50-16.10	**IL201**. *Alistair P. Rendell* Accelerating Quantum Chemistry Applications on Novel Computer Architectures	**IL202**. *Dimitrii Shalashilin* Multidimensional quantum mechanics with trajectory guided basis sets of Coherent States	**IL203**. *Notker Rösch* Scaling of properties of transition metal particles: a DFT study on Pd particles	**IL204**. *Chris Cramer* Metal ligand bonding and oxidation state: the curious case of the $[Cu_3S_2]^{3+}$ core	**IL205**. *Fernando Cossío* Computational studies on concerted and stepwise thermal cycloadditions
16.10-16.30	**IL206**. *Todd Martínez* Electronic structure and ab initio molecular dynamics on graphical processing units	**IL207**. *Satoshi Maeda* Finding Unexpected Reaction Pathways using Automated Reaction Route Finders	**IL208**. *Larry Curtiss* First principles studies of subnanometer effects on catalytic activity and selectivity	**IL209**. *Shigeru Nagase* Interesting bonds and structures provided by heavier main group elements and transition metals	**IL210**. *Zhi-Xiang Yu* A Computationally Designed and Experimentally Verified [(5+2)+1] Reaction and Its Application

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THURSDAY JULY 21 FACULTY OF MEDICINE

	ROOM A (AULA 4)	ROOM B (AULA 5)	ROOM C (AULA 7)	ROOM D (AULA 8)	ROOM E (SALÓN DE ACTOS)
16.30-16.50	**IL211**. *Duncan Poole* GPU Progress in Computational Chemistry and the role NVIDIA plays	**IL212**. *Antonio Varandas* Two quests: weakness of HO_3, and Jahn-Teller dynamics via a generalized Born-Oppenheimer theory	**IL213**. *Alex Timoshkin* From donor-acceptor complexes to nano structures	**IL214**. *Eric Clot* DFT study of the mechanism of palladium-catalyzed arylation of carboxylic esters	**IL215**. *Philippe Hiberty* Correlation between the diradical character of 1,3-dipoles and their reactivity toward ethylene and acetylene
16.50-17.00	**OC106**.*Michelle M. Kuttel* Coarse-grained simulation of multiprotein complexes using GPU accelerators	**OC107**. *Christian R. Evenhuis* Speeding up multi-state dynamics with interpolated potential surfaces	**OC108**. *Carmen Herrmann* Designing molecular spintronics devices in the coherent tunneling regime	**OC109**. *Pere Miró* Carbon dioxide reduction catalyzed by mono and dinuclear ruthenium complexes	**OC110**. *Ponnambalam Venuvanalingam* Imidozirconocene mediated ring cleavage of epoxides; evidences on bifunctional reactivity from DFT
17.00-17.10	**OC111**. *Ross C. Walker* Towards routine microsecond molecular dynamics simulations of proteins on commodity hardware: Extreme GPU acceleration of AMBER	**OC112**. *María Besora* Mechanistic possibilities for oxidative addition to palladium catalysts: cis or trans? Retention or inversion?	**OC113**. *Joonkyung Jang* Computer simulation of self assembly in dip-pen nanolithography	**OC114**. *Olalla Nieto* Homogeneous catalysis with just gold. A Mechanistic study	**OC115**. *Etienne Derat* Of the ortho effect in palladium/ norbornene-catalyzed reactions: a theoretical investigation

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THURSDAY JULY 21 FACULTY OF MEDICINE

	ROOM A (AULA 4)	ROOM B (AULA 5)	ROOM C (AULA 7)	ROOM D (AULA 8)	ROOM E (SALÓN DE ACTOS)
17.10-17.40	COFFEE BREAK				
17.40-19.30	**TH3.1** Ring Currents/ magnetism/NMR (Chair: *Gabriela Borosky*)	**TH3.2** Molecular Recognition/ isomerization in biomolecules (Chair: *Pedro A. Fernandes*)	TH3.5 Enzymatic Reactions (Chair: *Juan Frau*)	**TH3.4** Metallochemistry/ more on homogeneous catalysis (Chair: *Feliu Maseras*)	**TH3.3** Molecular Modeling/ Design/simulations (Chair: *Meredith JT Jordan*)
17.40-18.00	**IL216**. *Kenneth Ruud* Understanding the chemical bond: Magnetically induced currents in bond-breaking processes	**IL217**. *Jörg Grunenberg* Complexity in Molecular Recognition	**IL220**. *David Smith* The activation of coenzyme B_{12}	**IL219**. *Nathalie Guihéry* Theoretical treatment of magnetic anisotropy in mono- and bi-nuclear complexes	**IL218**. *Hans Lüthi* Quantum Chemical Data Archives in Support of Method Development and Molecular Modeling
18.00-18.20	**IL221**. *Paolo Lazzeretti* A new quantifier of magnetotropicity	**OC117**. *Sonsoles Martín-Santamaría* Molecular recognition processes in glycobiology. Some examples from the molecular modelling approach **OC122**. *Devesh Kumar* Theoretical study on the mechanism of the oxygen activation process in cysteine dioxygenase enzymes	**IL225**. *Shigehiko Hayashi* Molecular mechanisms of enzymatic catalysis in F_1-ATPase and α-amylase	**IL224**. *Michele Dupuis* Computational Molecular Electrocatalysis: Thermodynamics, Structure, and Dynamics in H_2 Oxidation and Evolution Molecular Catalysts	**IL223**. *Julia Rice* Using condensed phase quantum chemistry to obtain better charge models for classical simulations

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THURSDAY JULY 21 FACULTY OF MEDICINE

	ROOM A (AULA 4)	ROOM B (AULA 5)	ROOM C (AULA 7)	ROOM D (AULA 8)	ROOM E (SALÓN DE ACTOS)
18.20-18.40	**IL226**. *Michael Bülh* Modelling NMR Properties of Transition Metal Complexes in the Solid State	**IL222**. *Emanuele Paci* Determination of flexibility of polypeptides using a novel sampling method that preserves the kinetics	**IL230**. *Fahmi Himo* Quantum chemical modelling of enzymatic reactions	**IL229**. *Nino Russo* On the role of the metal in reactions catalyzed by metal containing enzymes	**IL228**. *Preston MacDougal* Volume-rendering in tandem with hyperwall technology for a new molecular visualization-based platform for drug design
18.40-19.00	**IL231**. *Magdalena Pecul* Calculations of nuclear magnetic resonance parameters of heavy metal compounds	**IL227**. *Antonio Fernández-Ramos* A theoretical study about the importance of the conformational flexibility and of tunneling in the isomerization reaction of previtamin D	**IL235**. *Oscar Ventura* Computational study of the Lipscomb and Lindskog reaction paths for hydrolytic Zn enzymes using the L_3ZnOH/CS_2 biomimetic systems	**IL234**. *Nora H. De Leeuw* Ab initio Molecular Dynamics simulations of the cooperative adsorption of hydrazine and water on copper surfaces: Implications for shape control of nanoparticles	**IL233**. *Venkatesan Subramanian* Exploring the changes in the structure of α-helical peptides adsorbed on to single walled carbon nanotube using classical molecular dynamics simulation

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THURSDAY JULY 21 FACULTY OF MEDICINE

	ROOM A (AULA 4)	ROOM B (AULA 5)	ROOM C (AULA 7)	ROOM D (AULA 8)	ROOM E (SALÓN DE ACTOS)
19.00-19.10	**OC116**. *Marie-Laure Bonnet* Comprehensive Boronate behaviour in $Mg(BH_4)_2$ from First Principles NMR Spectroscopy	**IL232**. *Toyokazu Ishida* Computational modeling of carbohydrate recognition in selectin complex	**OC120**. *Matthias Stein* Computational re-design of hydrogenase enzymes	**OC119**. *Hrant P. Hratchian* Revelations from reaction path following: is there more to transition metal catalysis than barrier height suppression?	**OC118**. *Laurence Leherte* Design of a reduced point charge model for proteins – molecular dynamics applications
19.10-19.20	**OC121**. *Dage Sundholm* Estimating molecular properties from magnetically induced current densities		**OC125**. *Pedro J. Silva* Reactivity of P450 cytochromes towards 1,2-dihydro-1,2-azaborine	**OC124**. *Gregori Ujaque* AIMD approach to transition metal catalyzed reactions in water	**OC123**. *Luca De Vico* A computational enzyme activity design of hiv-1 protease
19.20-19.30	**OC126**. *Mercè Deumal* Playing Molecule-based Magnets Quizzies: Unraveling Macroscopic Magnetic Behavior from a Microscopic Quantum Perspective	**OC127**. *Marco Marazzi* Ultrafast internal conversion as a possible mechanism of photostability in gamma-crystallin	**OC130**. *Jordi Poater* Analysis of the selectivity in the DNA replication mechanism through solvation, p-stacking and hydrogen bonding effects	**OC129**. *Julien A. Panetier* Catalytic hydrodefluorination of pentafluorobenzene by $[Ru(NHC)(PPh_3)_2(CO)H_2]$: theory explains the novel ortho-regioselectivity	**OC128**. *Katharina Meier* On the effect of a variation of the force field, spatial boundary condition and size of the QM region in QM/MM MD simulations

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FRIDAY JULY 22

9.00-11.00	**F1. Plenary Session (Chair: *Odile Eisenstein*)** **AUDITORIO DE GALICIA**
9.00-9.40	**PL7.** *Fred Manby.* Embedding as a new perspective on electronic structure theory
9.40-10.20	**PL8.** *Kimihiko Hirao.* Recent advances in LC-DFT
10.20-11.00	**PL9.** *Daniel Crawford.* Through the looking glass, and what the quantum chemist found there
11.00-11.30	**COFFEE BREAK**
11.30-13.30	**Poster Session III (PIII-1 TO PIII-267)** **FACULTY OF ECONOMY**
13.30-15.30	**LUNCH BREAK**
15.30-17.30	**F2. Plenary Session (Chair: Kangnian Fan)** **AUDITORIO DE GALICIA**
15.30-16.10	**PL10.** *Qiang Cui.* "Multi-scale" simulation of processes in membrane proteins and biomembranes: methods and applications
16.10-16.50	**PL11.** *Jesús Ugalde.* Natural Orbital Functional Theory and Implementation
16.50-17.30	**PL12.** *Peter Gill.* Improved DFT from electrons on a sphere
17.30-18.00	**F3. Closing Ceremony**
21,00	**BANQUET Pazo de San Lorenzo**

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