Programme IMAMPC 2014

	8 July	9 July	10 July	11 July
		Session 2	**Session 4**	**Session 6**
09:30 – 10:10		Lique, F. (S2_P1)	Akbar S. (S4_P1)	De Fazio, D. (S6_P1)
10:10 – 10:30		Bulut, N. (S2_01)	Dyke, J. (S4_O1)	Vila, A. (S6_O1)
10:30 – 10:50		Lanza, M. (S2_O2)	Schalk, O. (S4_O2)	Svodoba, O. (S6_O2)
10:50 – 11:20		**Coffee Break**	**Coffee Break**	**Coffee Break**
11:20 – 12:00		Le Picard, S. (S2_P2)	Ingrosso, F.(S4_P2)	Emilio Martínez (S6_P2)
12:00 – 12:20	Welcome &	Hernandez-Vera, M. (S2_03)	Marques, J. (S4_O3)	Woywod C. (S6_O3)
12:20 – 12:40	Registration	Sanz,C (S2_O4)	Roncero, O. (S4_O4)	Brandao J. (S6_O4)
12:40 – 13:00		Krasnokutskiy, S. (S2_O5)		**CLOSING**
13:00 – 15:00		**Lunch**	**Lunch**	**Lunch**
	Session 1	**Session 3**	**Session 5**	
15:00 – 15:40	Rosta, E. (S1_P1)	Graham, W. (S3_P1)	Narevicius, E. (S5_P1)	
15:40 – 16:00	Jambrina, P (S1_01)	Pelaez, D. (S3_O1)	Lara, M. (S5_O1)	
16:00 – 16:20	Oliveira L. F. L. (S1_02)	Arismendi, D. (S3_O2)	Chefdeville, S. (S5_O2)	
16:20 – 16:40	Pikulska, A. (S1_03)	Tandy, J. (S3_O3)	Zuchowski, P. (S5_O3)	
16:40 – 17:00	**Coffee Break**	**Coffee Break**	**Coffee Break**	
17:00 – 17:40	Duarte, F. (S1_P2)	Buchete, N. (S3_P2)	González, R. (S5_P2)	
17:40 – 18:00	Latimer, E. (S1_04)	Tapavicza, E. (S3_O4)	Leonardo, M (S5_P3)	
18:00 – 18:20	Piekarski D.G. (S1_05)	Suarez, J. (S3_O5)		
18:20 – 18:40				

S1: MACROMOLECULES

S2: ASTROCHEMISTRY

S3: THEORETICAL COMP. I

S4: THEORETICAL COMP. II

S5: COLD ATOMS AND MOLE

S6: REACTION DYNAM.

Session 1: Macromolecules and aggregates.		
S1_P1	Rosta, E.	Catalytic Mechanism of Phosphate Cleavage Reactions.
S1_P2	Duarte, F:	Phosphoryl and Related Group Transfer Reactions: Challenges in Interpreting Experimental and Theoretical Data.
S1_O1	Jambrina, P.	Computational Study of the phosphorylation of RAF dimers.
S1_O2	Oliveira, L. F. L.	Energetic and thermodynamic properties of protonated water clusters and water clusters adsorbed on polycyclic aromatic hydrocarbons.
S1_O3	Pikulska, A.	Calculations of circular dichroism and circularly polarized luminescence of biologically relevant chromophores.
S1_O4	Latimer, E.	Formation of novel nanoparticles in helium droplets.
S1_O5	Piekarski, D.G	Dynamics of excited doubly charged -alanine and neutral clusters of -alanine in the gas phase.
Session 2: Astrochemistry.		
S2_P1	Lique, F.	Collisional excitation of CN and O_2 by H_2: comparison of theory and experiments and astrophysical applications.
S2_P2	Le Picard, S.	Low temperature kinetics and astrophysical applications.
S2_O1	Bulut, N.	Studies of the F+DCl→Cl+DF reaction by using wave packet and time independent methods: isotope effects.
S2_O2	Lanza, M.	Is HCL really the main chlorine carrier in molecular clouds?.
S2_O3	Hernandez-Vera, M.	Rotational excitation of HCN by para- and ortho-H_2.
S2_O4	Sanz, C.	Quantum study and quasi-classical collisions of $H_2 + H_2^+$ reaction.
S2_O5	Krasnokutski, A.S	Ultra-Low-Temperature Reactions of C(^{3}PJ) Atoms with PAH Molecules in Helium Droplets and in the Interstellar Medium.
Session 3: Theoretical and Computational Chemistry I.		
S3_P2	Worth, G.	Multi-mode multi-state quantum dynamics for photo-excited polyatomic molecules: The Hamiltonian problem.

S3_P2	Buchete, N.	Coarse master equations for peptide folding and peptide-peptide interactions.
S3_O1	Pelaez, D.	Towards High Dimensional Quantum Dynamics with MCTDH.
S3_O2	Arismendi, D	Confining molecules inside a nanoscale cavity: the case of clathrate hydrates.
S3_O3	Tandy, J.	Dynamic and non-adiabatic effects in the stereocontrol of photoinduced electrocyclic reactions.
S3_O4	Tapavicza, E.	Probing Salt Solvation in Helium Droplets via Infrared Depletion Spectroscopy.
S3_O5	Suarez, J.	Non-adiabatic dynamical description of H_2O+(~B^2B_2) fragmentation.
Session 4: Theoretical and Computational Chemistry II.		
S4_P1	Akbar S.	Molecular QED theory of two- and three-body dispersion forces.
S4_P2	Ingrosso, F.	New Routes for Improved Solubility in Supercritical CO_2: When Theory Comes in Handy.
S4_O1	Dyke, J.	Reactive intermediates of atmospheric importance studied with photoionization and quantum chemistry calculations.
S4_O2	Schalk, O.	Time-resolved photoelectron spectroscopy and ab initio calculation on no/no2 release of nitroaromatics.
S4_O3	Marques, J.	Microsolvation aggregates of alkali-metal ions with aromatic rings.
S4_O4	Roncero, O.	A density-difference-driven optimized embedding potential method to study the spectroscopy of Br_2 in water clusters and clathrate cages.
Session 5: Cold atoms and molecules.		
S5_P1	Narevicius, E	Chemistry with Cold Molecules: from Universality to Quantum Resonances.
S5_P2	González, R	Controlling magnetic feshbach resonances and photoassociation rates with nonresonant light.
S5_P3	Leonardo, M.	Statistical product distributions for ultracold reactions in external fields.
S5_O1	Lara, M.	Universality in the cold and ultracold dynamics of the Barrierless reaction $D^+ + H_2$.

S5_O2	Chefdeville, S.	Observation of partial wave resonances in O_2-H_2 inelastic collisions at very low collision energy.
S5_O3	Żuchowski, P.	Formation of molecules with both magnetic and electric dipole moments.
Session 6: Reaction Dynamics.		
S6_P1	De Fazio, D.	The chemistry of the early universe: a comparison among dynamical approaches.
S6_P2	Martínez, E.	Energy transfer and thermal accommodation in gas-surface scattering.
S6_O1	Vilà, A	Photodissociation quantum dynamics of diatomic molecules in a quantum solvent (^{4}He nanodroplets).
S6_O2	Svodoba, O.	Atmospheric photodissociation of the nitrate anion.
S6_O3	Woywod, C.	Exact and approximate wave packet dynamics with quantum trajectories.
S6_O4	Brandao, J.	Following the OH radical in hidrogen combustion.
Posters		
P1	Bartolomei, M.	Water Passage through Graphynes' Pores: FirstPrinciples Penetration Barrier and Force Field Optimization.
P2	Bulut, N.	Height dependent integral cross-sections and rate coefficients for the O^++H_2 (v=0,j=0) reaction in the ionosphere.
P3	Prosmiti, R.	Stability of rare gas–water clusters under pressure: the Ar and Kr case.
P4	Rubešová, M.	Simulations of X-ray absorption spectra of ferrioxalate upon UV excitation.
P5	Aguado, A.	How many adiabatic states are needed for diabatization?.
P6	Oliveira, L.F.L.	Density functional theory study of water adsorption on IrO_2(110), RuO_2(110) and $Ru_xIr_{1-x}O_2$.
P7	Zanchet, A.	Theoretical study of the reaction of S^+ with vibrationally excited H_2.
P8	González-Martínez, M.	On the basis size problem in ultracold molecular scattering: Approximate hyperfine cross sections from hyperfine-free calculations.

P9	González, M.	Quantum dynamics of O+ $H_2^+ \rightarrow OH^+ + H$, $OH + H^+$. Influence of nonadiabatic effects.
P10	González, M.	Oxidation of atmospheric mercury by the OH radical. Ab initio and quasiclassical trajectory study.