Scientific Program – QUITEL2014								
	Sunday Nov 23rd	Monday Nov 24th	Tuesday Nov 25th	Wednesday Nov 26th	Thursday Nov 27th	Friday Nov 28th	Saturday Nov 29th	Sunday Nov 30th
8:00-8:45	Arrival to SCY	P-1A	Free	O-1C	Free	P-1E	Free	Departure from SCY
8:45-9:10		O-1A		O-2C		O-1E		
9:10-9:35		O-2A		O-3C		O-2E		
9:35-10:00		O-3A		O-4C		O-3E		
10:00-10:25		O-4A		O-5C		O-4E		
10:25-11:00		Break		Break		Break		
11:00-11:45		P-2A		P-1C		P-2E		
11:45-12:10		O-5A		O-6C		O-5E		
12:10-12:35		O-6A		O-7C		O-6E		
12:35-13:00		O-7A		O-8C		O-7E		
13:00-15:00		Lunch						
15:00-15:45	Registration	P-3A	P-1B	P-2C	P-1D	P-3E		
15:45-16:10	Inauguration Act	O-8A	O-1B	O-9C	O-1D	O-8E		
16:10-16:35		O-9A	O-2B	O-10C	O-2D	O-9E		
16:35-17:00	Opening Talk	O-10A	O-3B	O-11C	O-3D	O-10E		
17:00-17:25		O-11A	O-4B	O-12C	O-4D	O-11E		
17:25-18:00	Break					Closing Act		
18:00-20:00	Welcome Cocktail		Poster Session A	Poster Session B	Poster Session C			

Plenary conferences: 40 mins + 5 mins Q&A
Oral contributions: 20 mins + 5 mins Q&A
Lunch is not included in the inscription fee

List of Contributions

Plenary Conferences		
Opening	*From photosynthesis to sensors, solar cells and photovoltaics: How is theoretical chemistry helping us to understand how they work and control the design of devices*	V. Mujica
P-1A	*Recent advances in computa- tional proteomics.*	P. A. Fernandez
P-2A	*Theoretical study of the effect of heterogeneous medium in the electronic properties of molecules with biophysical interest.*	K. Coutinho
P-3A	*A new path for nanoparticles: Toward fully synthetic protein mimics and beyond.*	A. Alexander-Katz
P-1B	*Finding renewable-energy organic materials using high- throughput computational discovery approaches.*	A. Aspuru-Guzik
P-1C	*A new justification for hybrid functionals in DFT.*	E. V. Ludeña
P-2C	*N-representable 1-RDM Theory.*	M. Piris
P-1D	*Leveraging machine learning and stream processors for computa- tional chemistry.*	T. J. Martínez
P-1E	*Ab-initio methods for time- resolved attosecond dynamics of laser-driven many-electron molecules.*	T.T. Nguyen-Dang
P-2E	*The chemical bond overlap polar- izability and covalency. Concepts and applications: From diatomic molecules to solids.*	O. L. Malta
P-3E	*The "converse" method for the calculation of NMR and EPR pa- rameters: Theory and ab-initio calculations.*	D. Ceresoli
Oral Contributions		
O-1A	*Electronic and vibrational energy relaxation after photoexcitation in chlorophylls.*	S. Fernandez-Alberti
O-2A	*Electron-molecule collisions: The influence of microsolvation on the shape resonance spectra and on the differential cross sections.*	M.H.F. Bettega
O-3A	*Spin states along the catalytic cycle of non-heme Fe-containing enzymes.*	F.P. Cossío
O-4A	*Gap behavior of Fibonacci molecular nanowire based on CH_2 and SiH_2 radicals*	D.L. Azevedo
O-5A	*The reaction pathway leading to the formation of 2–aceto–2–hydroxybutyrate in the catalytic cycle of AHAS.*	E.J. Delgado
O-6A	*Finding reasons why two struc- tural related enzymes catalyze distinct reactions.*	G. Pierdominici-Sottile
O-7A	*Membrane binding of a curvature-sensing peptide of a lipid transport protein in yeast*	V. Monje-Galvan
O-8A	*Hybrid potential methods for the simulation of condensed phase reaction processes.*	M.J. Field
O-9A	*Complex physical chemical properties of water in nanospaces.*	C.I. Sainz-Díaz
O-10A	*Nanostructured clay minerals: A SCC-DFTB Study.*	H.A. Duarte
O-11A	*MRI contrast agents interacting with water molecules: Hierarchical clustering method for molecular dynamics data analysis.*	M.A. Méndez
O-1B	*Vibrationally induced dissociation of H_2SO_4*	J. Yosa
O-2B	*Intense laser induced ultrafast molecular processes: Imaging and control*	O. Atabek
O-3B	*DF-vdW vs. GGA functionals in methane adsorption on Ni surfaces.*	S. González
O-4B	*A Hopf bifurcation in a closed system under constant irradiation*	L.G. Arnaut

	and the onset of chemical oscillations	
O-1C	*How reliable is the hard-soft acid-base principle?*	C. Cárdenas
O-2C	*Tracking quantum control of arbitrary N-level systems.*	M.G.E. da Luz
O-3C	*Magnetic exchange couplings parameters from density functional theory calculations.*	J.E. Peralta
O-4C	*Studying positron binding with the any particle molecular orbital method*	A. Reyes
O-5C	*From P_{s2} to CH_4^+: A report on adiabatic vs non–adiabatic and normal-time vs extreme-time quantum regimes*	A.J.C. Varandas
O-6C	*Temperature and pressure effects on elastic and structural properties of minerals from Ab-initio simulations: The case of silicate garnets.*	A. Erba
O-7C	*Second derivatives and chemical descriptors: Advances and remarks*	R. C. Bochicchio
O-8C	*Intense field molecular photodissociation: The adiabatic views*	R. Lefebvre
O-9C	*Electronic structure of molecules in supercritical fluids*	S. Canuto
O-10C	*Molecular spectroscopy as a probe for quantum water potentials.*	C. Leforestier
O-11C	*Study of the antihypertensive ca- pacity of bioactive peptides using the QSAR computer model.*	A. Pérez
O-12C	*Electromagnetic study of the chlorosome antenna complex of Chlorobium tepidum*	S. Valleau
O-1D	*Interactions between precursors underlying the deposition of lucrative semiconductor materials: insights from theoretical calculations*	A. Kakanakova-Georgieva
O-2D	*Assessment of exchange– correlation functionals for calculating NMR coupling contants.*	J.M García de la Vega
O-3D	*New catalysts for CO2 activa- tion and hydrogenation based on Au/TiC and Cu/TiC: Theoretical modeling and experiments*	F. Illas
O-4D	*QCT studies on the dynamics of the F + CH_4 system performed on a new potential energy surface.*	J. Palma
O-1E	*Novel methyl-silyl-metal (H3C)nX(SiH3)3−n (X = B, Al, Ga, In) precursor molecules: Structure, reactivity, synthesis routes and identification by first-principles calculations*	G.K. Gueorguiev
O-2E	*Chiral discrimination via anapole magnetizabilities.*	M. Ferraro
O-3E	*How DFT computations can help in the design of new photosensitizers active in photodynamic therapy*	N. Russo
O-4E	*Some theoretical contributions concerning the physical chemistry properties of atmospheric media.*	J.C. Rayez
O-5E	*Experimental/theory coupling characterize transient species, understand and predict the behavior of molecules*	J.M. Sotiropoulos
O-6E	*Understanding the influence of terminal ligands on the electronic structure and bonding nature in $[Re_6(\mu_3\text{-}Q_8)]^{2+}$ clusters*	R. Arratia-Pérez
O-7E	*Electronic quenching in nitrogen atom-diatom collisions: Surface hopping dynamics and relevance for the atmosphere.*	B.R.I. Galvao
O-8E	*First principles based study of the surfaces and interfaces in lithium batteries: structure, elec- tronic properties and thermodynamic stability*	I. Baraille
O-9E	*A theoretical study of forma- tion routes and dimerization of methanimine and implications for the aerosols presence in the upper atmosphere of Titan*	M. Rosi
O-10E	*Quantum chemical approach to modeling binuclear metallohydrolase catalyzed reactions: The case of binuclear Co^{2+} OpdA enzyme*	M.E. Alberto
O-11E	*Highly active copper-ceria-titania catalysts. Insights from first principles calculations.*	J. Fdz. Sanz

Poster Contributions		
PP-1A	*Diffusion coefficients and intrinsic viscosity of PAMAM dendrimers.*	J. Alderete
PP-2A	*DFT study of catalysis dissociation of sodium nitrate ($NaNO_3$) on (533) and (577) irregular Cu,Pd and Rh surfaces.*	J. Bustamante
PP-3A	*Comparison of the reaction electronic flux and ETS-NOCV picture of the HCN→CNH isomerization reaction.*	S. Díaz
PP-4A	*Theoretical predictions of physicochemical properties of ionic liquids based-on bis(trifluoromethylsulfonyl)imide anion.*	J.M. García de la Vega
PP-5A	*Compactness of full configuration interaction wave functions: A seniority number approach.*	L. Lain
PP-6A	*Misfolding, metals and neurodegenerative diseases: XAS experiments and ab-initio simulations.*	S. Morante
PP-7A	*Revisiting the role of nucleophile, leaving group and solvent in backside S_N2 reactions ($Y^- + CH_3X \rightarrow YCH_3+X^-$; X,Y= F, Cl, Br, I): An atomic contribution study.*	L.M. Pedraza
PP-8A	*Predicting reactivity of 5– trifluoromethyluracil in gas and aqueous solution phases.*	R. Rudyk
PP-9A	*Hydrated ethanol dissociation mechanisms.*	A.F. Albernaz
PP-10A	*Study of resonance-assisted hydrogen bonds via magnetically induced currents.*	L. Alvarez-Thon
PP-11A	*Monte Carlo Adsorption affinity studio of modified nanomontmorillonite for the removal of chromate ions.*	A.C. Cadena
PP-12A	*Recombination dynamics between bipolarons and excitons in conjugated polymers.*	G. Magela e Silva
PP-13A	*Theoretical study of the geometric and electronic properties of theobromine.*	L.G. Santin
PP-14A	*The total position spread tensor in a molecular context.*	T. Leininger
PP-15A	*Relativistic theoretical study of the C–F bond activation mediated by lanthanide ions.*	J.A. Murillo-López
PP-16A	*Representation of potential energy surfaces and role of chiralityin weakly bound complexes: The hydrogen-peroxide-noble-gas interactions revisited.*	G.C. Possa
PP-17A	*Study of some simple approximations to the non-interacting kinetic energy functional.*	E.X. Salazar
PP-18A	*Molecular mechanics study of quercetin dimers in different conformations.*	A. Deriabina
PP-19A	*Oxidation and spin states in the cyclopropanation of alkenes catalyzed by Fe-porphirin catalysts.*	A. Arrieta
PP-20A	*Reliable computational model for nitrogen isotropic hyperfine coupling constants.*	P. Calle
PP-21A	*Ripping silicene: A theoretical study.*	B.G. Enders
PP-22A	*Highly reactive intermediates: Reaction mechanisms between substituted nitrenium ions and water.*	S. Gómez
PP-23A	*QSAR study of antioxidant activity of curcuminoids and analysis of their chemical reactivity under DFT.*	S. Llano
PP-24A	*Identification of binding mode of the epothilone-tubulin complex by molecular dynamics.*	K.R. Navarrete
PP-25A	*DFT and TD-DFT study of Lutetium bis-phthalocyanines: Electronic structure and spectroscopic properties.*	W.A. Rabanal-León
PP-26A	*Study of the effect of saponin Dioscin on the water–oil interface as a surfactant for enhanced oil recovery.*	S.K. Samaniego Andrade
PP-27A	*Water-methanol mixtures: Simulations of excess properties over the entire range of mole fractions.*	J.-C. Soetens
PP-28A	*Theoretical study of the reactivity of ionic hydrocarbons in gas phase.*	L. Baptista
PP-29A	*Study of the mechanism of carbocationic triple shift*	D.E. Ortega

	rearrangement.	
PP-30A	*Quantum chemical approach to modeling binuclear metallohydrolase catalyzed reactions: The case of binuclear Co^{2+} OpdA enzyme.*	M.E. Alberto
PP-31A	*DFG-out kinase inhibitors: Understanding their binding mechanism.*	J.M. Granadino-Roldan
PP-32A	*Ab-initio calculations of the thermodynamic properties of disubstituted diperoxides.*	C. Zambrano
PP-1B	*Theoretical study of amino disaccharides.*	A.J.L. Catao
PP-2B	*Curie temperature in double perovskites systems.*	O. Navarro
PP-3B	*Damage to DNA/RNA nucleobases by UV radiation and reactive oxygen species. II. OH radical addition and photochemistryof the hydroxylated products.*	D. Roca-Sanju´an
PP-4B	*Determination of geometric and electronic parameters of hydrazone using Car-Parrinello molecular dynamic.*	S.S. Oliveira
PP-5B	*Cluster origin of solvent features of C nanostructures.*	F. Torrens
PP-6B	*Design targeted drug carriers for potential use in cancer treatments.*	P. Barra
PP-7B	*Structural properties of a reverse inhibitor against the HIV virus, dideoxynucleoside zalcitabine in gas and aqueous solution phases.*	M.A. Checa
PP-8B	*DFT study of rutile and anatase materials doped with vanadium.*	J. Escobar
PP-9B	*Synthetic growth concept: A theoretical approach for designing novel nano-structured materials and low-dimensional phases.*	G.K. Gueorguiev
PP-10B	*Functionalizing carbon nanotubes to hold chemical reactions: A DFT study.*	A.L. Magalhaes
PP-11B	*Enthalpies of formation and acidities of thio- and selenobarbituric acids. A G3 and G4 study.*	R. Notario
PP-12B	*Diffusion of atoms and ions in solid state matrices.*	A.B. Rocha
PP-13B	*Geometrical functionalization of carbon nanotubes.*	J.F. Teixeira
PP-14B	*Structure of cetyltrimethylammonium bromide surfactant micellesfrom dissipative particle dynamics simulations.*	R. Paredes
PP-15B	*Evaluation of the CHARMM27 parameters by the topological study of G-Quadruplex.*	D. Barragán
PP-16B	*Solution vs. gas phase relative stability of the choline/acetylcholine 3iPO cavitand complexes: Mass spectrometry and theoretical studies.*	H. Chermette
PP-17B	*A novel class of polymers containing boron-boron triple bonds.*	F. Fantuzzi
PP-18B	*Theoretical study of the proton transfer in formamide and the role of the water molecule in the reaction.*	D. Guzmán-Angel
PP-19B	*A DFT study of complexes with two hyperjovinol a molecules binding to a Cu(II) ion.*	L. Mammino
PP-20B	*Structure and electronic properties of few-layer Pd films deposited on Re(0001) surface.*	J.E. Ontaneda-Rojas
PP-21B	*Molecular interactions between anionic dimethylphosphate and water.*	N. Rojas
PP-22B	*Configuration interaction wave functions based on the seniority number.*	A. Torre
PP-23B	*Theoretical investigation of the potential of metal-functionalized pyrogallol[4]arenes as molecular hydrogen storage materials.*	V. Posligua
PP-24B	*Analysis of key structural properties for a study group of intermolecular parallel Gquadruplexes X-ray and NMR structures simulated with molecular dynamics.*	M.L. Barreto Bermudez
PP-25B	*Adsorption of polycyclic aromatic pollutants on graphene, and effect of the structural defects and doping.*	D. Cortés-Arriagada
PP-26B	*Using nanoinformatic methods to automatically identify optimum polymerosomes for drug delivery applications.*	M.B. Ferraro

PP-27B	*Theoretical study of $N_2O \rightarrow N_2 + O$ reaction catalyzed by Odoped Pt_8 nanoparticles.*	E. Hernandez Vera
PP-28B	*Synergism between surfactants through mesoscopic dynamics to produce low interfacial tension at the hydrocarbon-water interface.*	J.A. Martiz Chalen
PP-29B	*Application of an orbital localization technique based on the topological analysis of the electron localization function.*	O.B. Oña
PP-30B	*Simulations of the absorption spectrum of crysteine modified gold nanoparticles in presence of TNT.*	P. Bonifassi
PP-31B	*Study of models for the structure of ecuadorian crude oil.*	S. Vaca
PP-1C	*Two-electron three-center (2e-3c) interactions in CH_4-Me^+ systems and simple X_4H^+ clusters.*	R.C. Bochicchio
PP-2C	*Docking studies of eugenyl acetate derivatives as new insect repellents.*	T.C.C. Franca
PP-3C	*β-Carotene encapsulation into single-walled Boron-nitride nanotubes: A theoretical study.*	A.L.A. Fonseca
PP-4C	*Reaction force and reaction flux analysis of proton transfers on DNA bases.*	B. Herrera
PP-5C	*Anisotropic and chemical agent effects on Fe-S bond stability of mechanically stressed rubredoxin.*	G.M. Arantes
PP-6C	*Ab initio and DFT study of chinesins I and II.*	L. Mammino
PP-7C	*Comparison of methallyl nickel complexes and their boron adducts in activation of ethylene: An explanation using dual descriptor of chemical reactivity.*	D.E. Ortega
PP-8C	*A theoretical study of formation routes and dimerization of methanimine and implications for the aerosols presence in the upper atmosphere of Titan.*	M. Rosi
PP-9C	*Deciphering the effect of fluorination of benzene in the chemical bond and its impact on the induced current densities and NICS.*	A. Vásquez-Espinal
PP-10C	*Spectroscopy, binding energy and properties calculations on silver and gold nanorods clusters: Staggered pentagonal (Ag_n for n=12 to 121) staggered cigare (Ag_n for n=12 to 120 and Au_n for n=12 to 120) and staggered hexagonal (Au_n n=14 to 74).*	P. Bonifassi
PP-11C	*Docking studies of DEET derivatives as new mosquitoes repellents.*	R. da S. Affonso
PP-12C	*Damage to DNA/RNA nucleobases by UV radiation and reactive oxygen species. I. Dissociation mechanisms caused by low energy electrons (0-3 eV).*	A. Francés-Monerris
PP-13C	*The mechanism of menshutkin reaction in gas and solvent phases from the perspective of the reaction electronic flux.*	R. Inostroza-Rivera
PP-14C	*A single-wall ZnO nanotube molecular modeling of β-Carotene encapsulation.*	F.F. Monteiro
PP-15C	*Theoretical study of the formation of acetyl intermediates over a cluster model of ZSM-5 zeolite.*	E.E. Ottavianelli
PP-16C	*Computational and experimental studies on β-Sheet breakers targeting $A\beta_{1-40}$ fibrils.*	G.C. Rossi
PP-17C	*A multiconfigurational approach for inner-shell states of liquid water.*	C.E.V. de Moura
PP-18C	*Hypertension therapy coming from computational enzymology.*	N.F. Brás
PP-19C	*Probing the ground and excited states of the HIO_2 isomers.*	G.L.C. de Souza
PP-20C	*Rh_6, Rh_{+6} and Rh_{-6} high reactivity to N_2O dissociation.*	H. Francisco-Rodríguez
PP-21C	*B_{18}^{2-}: The non-planar member of the Wankel Motor Family.*	R. Islas
PP-22C	*Mechanisms of retro-Diels Alder reaction of bicyclic organic compounds in the gas phase: Density functional Theory calculations.*	J.R. Mora

PP-23C	*Predicting the electronic structure and magnetic properties of UO_2^+, $[UO_2(CO)_5]^+$ and $[UO_2(Ar)_5]^+$ using wavefunction based methods.*	D. Páez Hernández
PP-24C	*Steered molecular dynamics and umbrella sampling approaches to the binding mechanism of DFGout p38α kinase inhibitors.*	J. Rubio-Martínez
PP-25C	*Resorcenarene cavitands as gas storage devices: A theoretical computational study.*	C. Zambrano
PP-26C	*Polar molecules engaged in pendular states captured by molecular beam scattering experiments.*	L.F. Roncaratti
PP-27C	*Assessing the importance of electron correlation: Study of trimethylamine – hydrogen halide pairs using Hartree-Fock and post Hartree-Fock methods.*	R.A. Cazar
PP-28C	*Computational modelling of copper complexes relevant to alzheimer disease.*	J. Alí-Torres
PP-29C	*Study of the trans-cis isomerization of quinolinyldiazenylbenzothiophene derivatives: Activation energy and stability.*	M. Rojas Poblete
PP-30C	*Molecular engineering methods applied to the efficient development of catalysts.*	F.J. Torres