WATOC 2014
5-10 October Santiago, Chile

10th Congress of the World Association of Theoretical and Computational Chemists

Advances in Electronic Structure Theory; Chemical Reactions and Catalysis; Time Dependent Phenomena; Ab Initio Quantum Chemistry; Spectroscopy; DFT; Advanced Materials; Spin; QM/MM; Energy Conversion and Storage...

WATOC Program for Sunday October 5, 2014

Timing	Sunday 5
14:00-20:00	Registration
16:00-16:40	Opening Ceremony
16:40-17:00	IC000
17:00-17:45	PL1
17:45-20:00	Chilean Dances & Welcome Cocktail

The registration desk will be open from 14:00, it will remain open until 20:00.

Opening Ceremony:
16:00-16:10: Words by Professor Ignacio Sanchez, President of PUC.
16:10-16:20: Words by the Dean of the Faculty of Chemistry at PUC, Prof. Bárbara Loeb.
16:20-16:30: Words from the Organizers, Professor Alejandro Toro-Labbé.
16:30-16:40: Words by the President of WATOC, Prof. Walter Thiel (Germany).

16:40-17:00: Invited Conference **IC000** by Professor Leo Radom (Australia): **The Tenth Congress of WATOC: Reflections on its Origins and Growth.**

17:00-17:45: Plenary Lecture **PL1** by Professor Manuel Yáñez (Spain): **From Old Bonding Patterns to New Enhanced Reactivity Trends.**

17:45-20:00: Break, Chilean Dances and Welcome Cocktail.

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WATOC Program for Monday 6 to Thursday 9

Timing	Monday 6	Tuesday 7	Wednesday 8	Thursday 9
8:30 -9:15	PL2	PL4	PL6	PL8
9:15-10:00	PL3	PL5	PL7	PL9
10:00-10:30	Coffe Break	Coffe Break	Coffe Break	Coffe Break
10:30-10:55	IC001-005	IC046-050	IC091-095	IC121-125
10:55-11:20	IC006-010	IC051-055	IC096-100	IC126-130
11:20-11:45	IC011-015	IC056-060	IC101-105	IC131-135
11:45-12:10	IC016-020	IC061-065	IC106-110	IC136-140
12:10-12:35	Lunch	Lunch	IC111-115	Lunch
12:35-13:00	&	&	IC116-120	&
13:00-13:25 13:25-13:50 13:50-14:15	Posters Session 1 (PP001-PP190)	Posters Session 2 (PP191-PP376)		Poster Session 3 (PP377-PP568)
14:15-14:40	IC021-025	IC066-070	FREE AFTERNOON	IC141-145
14:40-15:05	IC026-030	IC071-075		IC146-150
15:05-15:30	IC031-035	IC076-080		IC151-155
15:30-15:55	IC036-040	IC081-085		IC156-160
15:55-16:20	IC041-045	IC086-090		IC161-165
16:20-16:40	Coffe Break	Coffe Break		Coffe Break
16:40-16:55	OP001-005	OP031-035		OP061-065
16:55-17:10	OP006-010	OP036-040		OP066-070
17:10-17:25	OP011-015	OP041-045		OP071-075
17:25-17:40	OP016-020	OP046-050		OP076-080
17:40-17:55	OP021-025	OP051-055		OP081-085
17:55-18:10	OP026-030	OP056-060		OP086-090
18:10-19:30	Poster Session 1 (PP001-PP190)	Poster Session 2 (PP191-PP376)		Poster Session 3 (PP377-PP568)
19:30-22:00				WATOC 2014 Dinner

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WATOC Program for Friday October 10, 2014

Timing	Friday 10
8:30-9:15	PL10
9:15-10:00	PL11
10:00-10:30	Coffe Break
10:30-10:55	IC166-170
10:55-11:20	IC171-175
11:20-11:45	IC176-180
11:45-12:10	IC181-185
12:10-12:35	Lunch
12:35-13:00	
13:00-13:25	
13:25-13:50	IC186-190
13:50-14:15	IC191-195
14:15-14:40	IC196-200
14:40-14:55	OP091-095
14:55-15:10	OP096-100
15:10-15:25	OP101-105
15:25-15:40	OP106-110
15:40-16:30	Closing Ceremony

Special Sessions:

In Memoriam of the late Professor Rubén Contreras: Monday 06, 14:45-16:20, Room 4. **Chair: Gustavo E. Scuseria (USA).**

Session celebrating 50 years of the Hohenberg-Kohn Theorems: Wednesday 08, 10:30-13:00, Room 1. **Chair: Prof. Paul Geerlings (Belgium).**

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WATOC 2014: Plenary Lectures (PL)*

Lecture	Date	Title	Lecturer
PL1	SUNDAY 5 17:00	From Old Bonding Patterns to New Enhanced Reactivity Trends	Manuel Yáñez (Spain)
PL2	MONDAY 6 8:30AM	Concepts for Organizing Chemical Knowledge	Paul W. Ayers (Canada) 2012 Dirac Medal.
PL3	MONDAY 6 9:15AM	Fragmentation: A Route to Accurate Calculation on Large Molecular Systems	Mark Gordon (USA) 2014 Schrödinger Medal,
PL4	TUESDAY 7 8:30AM	(Photo)Electrocatalysis: Theory and Mechanisms of Charge Transfer at Metal Surfaces	Emily Carter (USA)
PL5	TUESDAY 7 9:15AM	Multiscale Modeling of Complex Biological Systems and Processes	Arieh Warshel (USA)
PL6	WEDNESDAY 8 8:30AM	Optical Spectra with Time-Dependent Density Functional Theory	Denis Jacquemin (France) 2014 Dirac Medal
PL7	WEDNESDAY 8 9:15AM	Modeling of Complex Chemical Processes by Dispersion-Corrected DFT	Stefan Grimme (Germany) 2013 Schrödinger Medal
PL8	THURSDAY 9 8:30AM	From One to Many-Electrons Chemical Bonds	Marco A. Chaer Nascimento (Brazil)
PL9	THURSDAY 9 9:15AM	A Variational Approach to Enhanced Sampling and Free Energy Calculations	Michele Parrinello (Switzerland)
PL10	FRIDAY 10 8:30AM	New Tools for Ab Initio Molecular Electronic Structure Calculations of Ground and Excited States	Filipp Furche (USA) 2013 Dirac Medal
PL11	FRIDAY 10 9:15AM	Relativistic Quantum Chemistry: The Broad Picture and Some Recent Results	Pekka Pyykkö (Finland) 2012 Schrödinger Medal

***All Plenary Lectures will be presented in Room 2**

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INVITED CONFERENCES

IC Code	Speaker	Country	Title	Day	Time	Room
IC000	Leo Radom	Australia	The tenth congress of WATOC: reflections on its origins and growth	Sun 05	16:40-17:00	Room 2
IC001	Tomasz Wesolowski	Switzerland	Multi-level simulation methods for electronic structure based on frozen-density embedding theory	Mon 06	10:30-10:55	Room 1
IC002	Ajit Thakkar	Canada	Simple relationships among molecular properties	Mon 06	10:30-10:55	Room 2
IC003	Tim Clark	Germany	Modeling organic electronic devices.	Mon 06	10:30-10:55	Room 3
IC004	Antonio J.C. Varandas	Portugal	From PS2 to H3+, HO3-, and CH4+: a tale of accurate electronic structure and quantum dynamics calculations	Mon 06	10:30-10:55	Room 4
IC005	Attila G. Csaszar	Hungary	On nuclear motion in HN+ (n = 2, 3, 5) systems.	Mon 06	10:30-10:55	Room 5
IC006	Carlo Adamo	France	Hybrid and double-hybrid parameter-free functionals.	Mon 06	10:55-11:20	Room 1
IC007	Laurent Joubert	France	Halogen bonds: measuring the sigma hole.	Mon 06	10:55-11:20	Room 2
IC008	Eluvathingal D. Jemmis	India	Perspectives on the structure, bonding and reactivity of metallacyclocumulenes.	Mon 06	10:55-11:20	Room 3
IC009	Gerardo Delgado-Barrio	Spain	Vibrational dynamics and spectral simulations of the fluxional h5+ cation and its isotopologues.	Mon 06	10:55-11:20	Room 4
IC010	Albert Rimola	Spain	Computational study on the formation of H2 and CH3OH on surfaces of interstellar dust particles.	Mon 06	10:55-11:20	Room 5

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IC011	Xin Xu	PR China	Construction of a parameter–free doubly hybrid density functional from adiabatic connection.	**Mon 06**	**11:20-11:45**	**Room 1**
IC012	J. Raúl Alvarez-Idaboy	Mexico	On the importance of using appropriate models to study reactions in solution, application to oxidative stress processes.	**Mon 06**	**11:20-11:45**	**Room 2**
IC013	Minh Tho Nguyen	Belgium	Non-classical aromaticity of clusters.	**Mon 06**	**11:20-11:45**	**Room 3**
IC014	Alexandre A. Leitão	Brazil	Using DFT calculations for NMR simulations as a tool to understand structure of materials.	**Mon 06**	**11:20-11:45**	**Room 4**
IC015	Patricio Fuentealba	Chile	Coulomb explosion in atomic clusters. an ab initio molecular dynamic study.	**Mon 06**	**11:20-11:45**	**Room 5**
IC016	Roland Lindh	Sweden	Analytical RI/CD-SA-CASSCF gradients.	**Mon 06**	**11:45-12:10**	**Room 1**
IC017	Dennis Salahub	Canada	Towards the multiscale modeling of chemical reactions in complex environments.	**Mon 06**	**11:45-12:10**	**Room 2**
IC018	Miquel Solà	Spain	Aromaticity in fullerenes and endohedral metallofullerenes. Effects on molecular structure and reactivity.	**Mon 06**	**11:45-12:10**	**Room 3**
IC019	Jiri Vanicek	Switzerland	Efficient on-the-fly ab initio method for computing nonadiabatic electronic spectra.	**Mon 06**	**11:45-12:10**	**Room 4**
IC020	Daniel P. Vercauteren	Belgium	A multiscale study of the mu opioid receptor flexibility. Atomistic, coarse-grained, cross-grained, and multi-grained models.	**Mon 06**	**11:45-12:10**	**Room 5**

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IC021	Michel Caffarel	France	.Systematic improvement of nodes in qmc using perturbatively selected configuration interaction.	**Mon 06**	**14:15-14:40**	**Room 1**
IC022	Sason Shaik	Israel	New aspects in bonding and reactivity.	**Mon 06**	**14:15-14:40**	**Room 2**
IC023	An Ghysels	Belgium	Critical analysis of liquid structure models	**Mon 06**	**14:15-14:40**	**Room 3**
IC024	Gustavo Aucar	Argentina	Magnetic properties in heavy-atom containing molecules.	**Mon 06**	**14:15-14:40**	**Room 4**
IC025	Andres Reyes	Colombia	Using the any particle molecular orbital method to study proton and positron binding.	**Mon 06**	**14:15-14:40**	**Room 5**
IC026	William A. Lester, Jr	USA	Some recent developments and applications of QMC to the electronic structure of molecules.	**Mon 06**	**14:40-15:05**	**Room 1**
IC027	G. Narahari Sastry	India	Cooperativity of non-covalent interactions.	**Mon 06**	**14:40-15:05**	**Room 2**
IC028	Suresh Cherumuttathu	India	Hypervalent carbon in alkene metathesis and planar tetravalent carbon in alkyne metathesis.	**Mon 06**	**14:40-15:05**	**Room 3**
IC029	Jiri Pittner	Czech Republic	Molecular dynamics with non-adiabatic and spin-orbit effects.	**Mon 06**	**14:40-15:05**	**Room 4**
IC030	Xavier Assfeld	France	Electronic excited states of biomolecules.	**Mon 06**	**14:40-15:05**	**Room 5**
IC031	T. Daniel Crawford	USA	On the non-locality of higher-order molecular properties: a challenge for reduced-scaling models.	**Mon 06**	**15:05-15:30**	**Room 1**
IC032	Russell Boyd	Canada	Insight into hydrogen-bonded clusters and noncovalent interactions from changes in atomic energies.	**Mon 06**	**15:05-15:30**	**Room 2**

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IC033	Helio Anderson Duarte	Brazil	Reactivity of the sulfide mineral surfaces - a DFT study.	**Mon 06**	**15:05-15:30**	**Room 3**
IC034	Vladimiro Mujica	USA	Molecular spin filters.	**Mon 06**	**15:05-15:30**	**Room 4**
IC035	Mario Barbatti	Germany	Photoinduced processes in nucleic acids.	**Mon 06**	**15:05-15:30**	**Room 5**
IC036	Mario Piris	Spain	Interacting pairs in natural orbital functional theory.	**Mon 06**	**15:30-15:55**	**Room 1**
IC037	Tore Brinck	Sweden	Analyzing halogen bonds and other non-covalent interactions using computed molecular surface properties.	**Mon 06**	**15:30-15:55**	**Room 2**
IC038	Joachim Sauer	Germany	Ab initio free energy calculations with chemical accuracy for molecule - surface interactions.	**Mon 06**	**15:30-15:55**	**Room 3**
IC039	Ramiro Arratia-Pérez	Chile	Relativistic studies of the intermetallic bond and optical properties in diatomics and in 5d-4(5)f complexes.	**Mon 06**	**15:30-15:55**	**Room 4**
IC040	Anastassia Alexandrova	USA	In silico design of metalloenzymes.	**Mon 06**	**15:30-15:55**	**Room 5**
IC041	Trygve Helgaker	Norway	Differentiable but exact formulation of density-functional theory.	**Mon 06**	**15:55-16:20**	**Room 1**
IC042	Joel M. Bowman	USA	Ab initio potential energy surfaces developed and employed in reaction dynamics calculations.	**Mon 06**	**15:55-16:20**	**Room 2**
IC043	Yitzhak Apeloig	Israel	Donor-acceptor adducts of aminocarbenes with silylenes. Scaling computationally the acceptor ability of the carbenes and predicting the synthesis of novel silenes.	**Mon 06**	**15:55-16:20**	**Room 3**

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IC044	Adriana B. Pierini	Argentina	New insights to interpret the chemistry of species formed by electron transfer (ET): radical and radical anions.	**Mon 06**	**15:55-16:20**	**Room 4**
IC045	Vicent Moliner	Spain	Computational design of new biological catalysts. Role of protein motions to catalysis.	**Mon 06**	**15:55-16:20**	**Room 5**
IC046	Paul Geerlings	Belgium	Conceptual density functional theory: chemistry from the linear response function.	**Tue 07**	**10:30-10:55**	**Room 1**
IC047	Josep M. Oliva	Spain	Quantum chemistry and boron: the synergy of the forgotten element.	**Tue 07**	**10:30-10:55**	**Room 2**
IC048	Itamar Borges Jr.	Brazil	Energetic materials: ground and excited state properties.	**Tue 07**	**10:30-10:55**	**Room 3**
IC049	Ria Broer	Netherlands	Spin crossover in Fe(II) metal-organic complexes.	**Tue 07**	**10:30-10:55**	**Room 4**
IC050	Mariona Sodupe	Spain	Photophysics of fluorescent markers for amyloid fibril detection.	**Tue 07**	**10:30-10:55**	**Room 5**
IC051	Samantha Jenkins	PR China	Conceptual quantum topology.	**Tue 07**	**10:55-11:20**	**Room 1**
IC052	Gernot Frenking	Germany	Bonding analysis of donor-acceptor complexes.	**Tue 07**	**10:55-11:20**	**Room 2**
IC053	Notker Rösch	Germany	Modeling biomass transformations over transition metals.	**Tue 07**	**10:55-11:20**	**Room 3**
IC054	Ilaria Ciofini	France	Photophysical properties of molecular compounds : insights from density functional theory.	**Tue 07**	**10:55-11:20**	**Room 4**

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IC055	Kevin Naidoo	South Africa	Reaction dynamics methods to accurately simulate chemical glycobiology events.	**Tue 07**	**10:55-11:20**	**Room 5**
IC056	Akitomo Tachibana	Japan	Electronic stress tensor of chemical bond.	**Tue 07**	**11:20-11:45**	**Room 1**
IC057	Michael B. Hall	USA	Mechanism of electrocatalytic purification of olefins by metal bis(dithiolenes).	**Tue 07**	**11:20-11:45**	**Room 2**
IC058	Julia Contreras-Garcia	France	Understanding the fundamental role of dispersion interactions in shaping carbon-based materials.	**Tue 07**	**11:20-11:45**	**Room 3**
IC059	Jesus Maria Ugalde	Spain	Quantum dot photoactivation by electron transfer. Insights form DFT and TDDFT calculations.	**Tue 07**	**11:20-11:45**	**Room 4**
IC060	Esteban Vöhringer-Martinez	Chile	The enzyme catalysis mechanism of PIN1: a mean reaction force study with improved electrostatics through dynamic Hirshfeld charges.	**Tue 07**	**11:20-11:45**	**Room 5**
IC061	Ángel Martín Pendás	Spain	A probabilistic foundation for the theory of chemical bonding.	**Tue 07**	**11:45-12:10**	**Room 1**
IC062	William L. Hase	USA	Non-statistical and non-IRC post-transition state chemical reaction dynamics.	**Tue 07**	**11:45-12:10**	**Room 2**
IC063	Karine Costuas	France	Multifunctional coordination complexes for molecular electronics and opto-electronics: a computational contribution.	**Tue 07**	**11:45-12:10**	**Room 3**

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IC064	Chantal Daniel	France	Photophysics of transition metal complexes: spin-orbit and environment effects.	**Tue 07**	**11:45-12:10**	**Room 4**
IC065	Henry Chermette	France	DFT as a tool for elucidating mass spectra.	**Tue 07**	**11:45-12:10**	**Room 5**
IC066	Gustavo E. Scuseria	USA	Unconventional Coupled Cluster Theories for Strong and Weak Correlations.	**Tue 07**	**14:15-14:40**	**Room 1**
IC067	Elfi Kraka	USA	New features of the unified reaction valley approach - from simple exchange reactions to homogenous catalysis	**Tue 07**	**14:15-14:40**	**Room 2**
IC068	Masahiro Ehara	Japan	Au and Au/Pd nanocluster catalysts.	**Tue 07**	**14:15-14:40**	**Room 3**
IC069	Sambhu Nath Datta	India	On theoretical design of magnetic organic molecules.	**Tue 07**	**14:15-14:40**	**Room 4**
IC070	Célia Fonseca Guerra	Netherlands	Resonance-assisted halogen bonds in N-halo-guanine quartets.	**Tue 07**	**14:15-14:40**	**Room 5**
IC071	Piotr Piecuch	USA	Combining active-space coupled-cluster approaches with moment energy corrections via the CC(P;Q) methodology.	**Tue 07**	**14:40-15:05**	**Room 1**
IC072	Pablo Jaque	Chile	Synchronicity in multi-bond chemical reactions: a reaction force constant analysis.	**Tue 07**	**14:40-15:05**	**Room 2**

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IC073	Zygmunt Flisak	Poland	Cocatalysts as reducing agents and the source of counter anions in coordinative olefin polymerization: a theoretical study.	**Tue 07**	**14:40-15:05**	**Room 3**
IC074	Regis Gautier	France	Density functional theory calculations of nuclear magnetic parameters of transition metal nuclei in solids.	**Tue 07**	**14:40-15:05**	**Room 4**
IC075	Marcelo Galván	Mexico	Dispersion cooperative effects in the stabilization energy of formic acid and L-cystine crystals.	**Tue 07**	**14:40-15:05**	**Room 5**
IC076	Sourav Pal	India	Cluster expansion methods for electronic structure and properties of molecules.	**Tue 07**	**15:05-15:30**	**Room 1**
IC077	Andreas Köster	Mexico	The electronic origin of the geometrical shell closing in Na55+.	**Tue 07**	**15:05-15:30**	**Room 2**
IC078	Hans Lischka	USA	The fascinating manifold of polyradical defect structures in graphene nanoflakes: a theoretical study.	**Tue 07**	**15:05-15:30**	**Room 3**
IC079	Marco Garavelli	France	Photoinduced dynamics in visual rhodopsins: a computational insight.	**Tue 07**	**15:05-15:30**	**Room 4**
IC080	Kwang S. Kim	Korea	Two dimensional molecular electronics spectroscopy for molecular fingerprinting and dna sequencing.	**Tue 07**	**15:05-15:30**	**Room 5**
IC081	Peter Pulay	USA	Efficient calculation of triple substitutions on coupled cluster theory.	**Tue 07**	**15:30-15:55**	**Room 1**
IC082	Teresa Head-Gordon	USA	Advanced potential energy surfaces for condensed phase simulation.	**Tue 07**	**15:30-15:55**	**Room 2**
IC083	Hans Peter Luthi	Switzerland	From “how it works” to “what works”: searching to develop novel cross-conjugated materials.	**Tue 07**	**15:30-15:55**	**Room 3**

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IC084	Wei-Hai Fang	PR China	Ab initio based non-adiabatic dynamics simulations on photodissociation of carbonyl compounds and photo-triggered helix-coil transition for a peptide.	**Tue 07**	**15:30-15:55**	**Room 4**
IC085	Jaroslav Burda	Czech Republic	Interaction of metallodrugs with models of DNA.	**Tue 07**	**15:30-15:55**	**Room 5**
IC086	Petr Carsky	Czech Republic	Efficient evaluation of exchange integrals and their derivatives by means of fourier transform of the 1/r operator and its numerical quadrature.	**Tue 07**	**15:55-16:20**	**Room 1**
IC087	Ricardo Longo	Brazil	Dynamics of chemical reactions.	**Tue 07**	**15:55-16:20**	**Room 2**
IC088	Joao B. L. Martins	Brazil	Adsorption of CO2 and coverage effects on zinc oxide surface.	**Tue 07**	**15:55-16:20**	**Room 3**
IC089	Peter Gill	Australia	Single-determinant models of excited states.	**Tue 07**	**15:55-16:20**	**Room 4**
IC090	Stefan Erhardt	UK	Computational investigation of a platinated DNA zinc finger complex.	**Tue 07**	**15:55-16:20**	**Room 5**
IC091	Melvyn P. Levy	USA	On variational principles in ground-state density-functional theory.	**Wed 08**	**10:30-10:55**	**Room 1**
IC092	Henry Rzepa	UK	Ten years on for the Houk-list transition states for organocatalysis and NCI analysis.	**Wed 08**	**10:30-10:55**	**Room 2**
IC093	Jon Mattin Matxain	Spain	Novel solid phases by self-assembling of nanoclusters.	**Wed 08**	**10:30-10:55**	**Room 3**

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IC094	Bogumil Jeziorski	Poland	Relativistic and quantum electrodynamics effects for frequency dependent polarizability and refractivity of helium.	**Wed 08**	**10:30-10:55**	**Room 4**
IC095	Pedro A Fernandes	Portugal	Computational proteomics cocktail.	**Wed 08**	**10:30-10:55**	**Room 5**
IC096	Weitao Yang	USA	Exchange-correlation and electronic excitation energies from pairing matrix fluctuations.	**Wed 08**	**10:55-11:20**	**Room 1**
IC097	Evert Jan Meijer	Netherlands	Modeling catalysis in aqueous solution.	**Wed 08**	**10:55-11:20**	**Room 2**
IC098	Aleksandar Staykov	Japan	Immobilizing metal nanoparticles on single wall nanotubes. Effect of surface curvature.	**Wed 08**	**10:55-11:20**	**Room 3**
IC099	Yoon Sup Lee	Korea	Multi-configuration spin-orbit calculations with two-component spinors and relativistic effective core potentials.	**Wed 08**	**10:55-11:20**	**Room 4**
IC100	Marta Ferraro	Argentina	Prediction of pharmaceutical crystal structures: a quantum espresso implementation with genetic algorithms.	**Wed 08**	**10:55-11:20**	**Room 5**
IC101	Rodney Bartlett	USA	Making Kohn-Sham DFT give the right answer for the right reason.	**Wed 08**	**11:20-11:45**	**Room 1**
IC102	Oscar L. Malta	Brazil	The chemical bond overlap polarizability and covalency concepts and applications: from diatomic molecules to solids.	**Wed 08**	**11:20-11:45**	**Room 2**

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IC103	Nino Russo	Italy	Theoretical study on catalytic generation, transport and storage of hydrogen for mobile applications.	**Wed 08**	**11:20-11:45**	**Room 3**
IC104	Joseph Vincent Ortiz	USA	Orbital concepts in spectra, energetics and transport from electron propagator theory.	**Wed 08**	**11:20-11:45**	**Room 4**
IC105	Tiziana Marino	Italy	Promiscuous activity of human carbonic anhydrase. A QM and QM/MM investigation.	**Wed 08**	**11:20-11:45**	**Room 5**
IC106	Henry F. Schaefer	USA	Density cumulant functional theory from a unitary transformation: N-representability, three-particle correlation effects, and application to O+4.	**Wed 08**	**11:45-12:10**	**Room 1**
IC107	Artur Michalak	Poland	Theoretical description of chemical bonding based on natural orbitals for chemical valence (NOCV).	**Wed 08**	**11:45-12:10**	**Room 2**
IC108	Miroslav Urban	Slovakia	Bonding character of small Au clusters with lone pair ligands.	**Wed 08**	**11:45-12:10**	**Room 3**
IC109	Christel M. Marian	Germany	Spin-forbidden molecular excited-state processes.	**Wed 08**	**11:45-12:10**	**Room 4**
IC110	Chaoyuan Zhu	Taiwan	Trajectroy-based nonadiabatic molecular dynamics without calculating nonadiabatic coupling vector.	**Wed 08**	**11:45-12:10**	**Room 5**
IC111	José Luis Gázquez	France	An accurate exchange GGA functional with correct asymptotic behavior in its exchange potential.	**Wed 08**	**12:10-12:35**	**Room 1**

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IC112	Christophe Morell	France	Dual descriptor: new physical bases and recent applications.	**Wed 08**	**12:10-12:35**	**Room 2**
IC113	Alejandro Ramirez-Solis	Mexico	The epsilon-dzeta phase transition in solid oxygen. Periodic ab initio and DFT studies with gaussian atomic basis sets.	**Wed 08**	**12:10-12:35**	**Room 3**
IC114	Jean Maruani	France	The Dirac electron as a massless charge spinning at light speed and the kinetic foundation of rest mass.	**Wed 08**	**12:10-12:35**	**Room 4**
IC115	Gerrit C. Groenenboom	Netherlands	Ab initio calculation of collisional and spectroscopic molecular properties for astrochemical and atmospheric applications.	**Wed 08**	**12:10-12:35**	**Room 5**
IC116	Matthias Ernzerhof	Canada	A first-principles correlation energy functional compatible with exact exchange.	**Wed 08**	**12:35-13:00**	**Room 1**
IC117	Pratim K. Chattaraj	India	Quantum potential based approaches towards quantum dynamics.	**Wed 08**	**12:35-13:00**	**Room 2**
IC118	Enrique Sanchez Marcos	Spain	Combining computer simulations with X-ray absorption spectroscopy in the study of trivalent actinide and lanthanide cations in aqueous solution.	**Wed 08**	**12:35-13:00**	**Room 3**
IC119	Josef Michl	Czech Republic	Singlet fission: the chromophores and their coupling.	**Wed 08**	**12:35-13:00**	**Room 4**
IC120	Lynn Kamerlin	Sweden	Chemically driven protein evolution among enzymes that catalyze phosphoryl transfer.	**Wed 08**	**12:35-13:00**	**Room 5**

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IC121	Christian Ochsenfeld	Germany	Fast quantum-chemical methods for large molecules: from intermolecular interactions to response properties.	**Thu 09**	**10:30-10:55**	**Room 1**
IC122	Albeiro Restrepo	Colombia	Mechanistic studies of the Wittig reaction.	**Thu 09**	**10:30-10:55**	**Room 2**
IC123	Zdenek Havlas	Czech Republic	Design of single fission structures: minimalist diabatic approach including overlap.	**Thu 09**	**10:30-10:55**	**Room 3**
IC124	Akihiro Morita	Japan	Theory and computational analysis of surface nonlinear spectroscopy.	**Thu 09**	**10:30-10:55**	**Room 4**
IC125	Johannes Kästner	Germany	Quantum mechanical tunneling of atoms in astrochemical reactions.	**Thu 09**	**10:30-10:55**	**Room 5**
IC126	Jorge Garza	Mexico	Analyzing quantum chemistry scalar fields by using GPUs.	**Thu 09**	**10:55-11:20**	**Room 1**
IC127	Willian Rocha	Brazil	DFT studies on the C-H bond activation of methane by transition metal compounds.	**Thu 09**	**10:55-11:20**	**Room 2**
IC128	Sylvio Canuto	Brazil	Electronic structure of atoms and molecules in supercritical fluids.	**Thu 09**	**10:55-11:20**	**Room 3**
IC129	Claude Pouchan	France	IR spectra of complex systems from DFT methods: the case of micro-hydrated molecular clusters.	**Thu 09**	**10:55-11:20**	**Room 4**
IC130	Marcelo Kogan	Chile	Gold nanoparticles functionalized with peptides for drug delivery, therapy and diagnosis.	**Thu 09**	**10:55-11:20**	**Room 5**
IC131	Anna Krylov	USA	Metastable Electronic States and Complex Variable Approaches: A Fresh Look at the Old Challenge.	**Thu 09**	**11:20-11:45**	**Room 1**

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INVITED CONFERENCES

IC132	Gabriel Merino	Mexico	Two stories about non-classical carbocations.	**Thu 09**	**11:20-11:45**	**Room 2**
IC133	Jinlong Yang	PR China	Novel sunlight driven photocatalysts for water splitting from first principles calculations.	**Thu 09**	**11:20-11:45**	**Room 3**
IC134	Jochen Autschbach	USA	In silico determination of spectroscopic parameters for molecules with elements across the periodic table.	**Thu 09**	**11:20-11:45**	**Room 4**
IC135	Antonio Largo	Spain	Possible ion-molecule reactions leading to interstellar glycine.	**Thu 09**	**11:20-11:45**	**Room 5**
IC136	Bernard Kirtman	USA	Electronic and nuclear response properties of infinite periodic systems in oscillating fields.	**Thu 09**	**11:45-12:10**	**Room 1**
IC137	Peter R. Schreiner	Germany	Carbonic acid revisited.	**Thu 09**	**11:45-12:10**	**Room 2**
IC138	Gregory Tschumper	USA	Benchmark vibrational frequencies for hydrogen bonding in water clusters and explicitly hydrated systems.	**Thu 09**	**11:45-12:10**	**Room 3**
IC139	Takao Tsuneda	Japan	Orbital energy gaps vs excitation energies for extended systems.	**Thu 09**	**11:45-12:10**	**Room 4**
IC140	Robert Benny Gerber	Israel	Unraveling mechanisms of important atmospheric reactions by ab initio molecular dynamics.	**Thu 09**	**11:45-12:10**	**Room 5**
IC141	Mark Hoffmann	USA	Advances in GVVPT2 multireference perturbation theory. Transition metals.	**Thu 09**	**14:15-14:40**	**Room 1**
IC142	Patrizia Calaminici	Mexico	Transition state search of finite systems.	**Thu 09**	**14:15-14:40**	**Room 2**
IC143	Masataka Nagaoka	Japan	Toward controlling complex chemical reactions in the 'molecular aggregation states' -from multiscale simulation to computational molecular technology.	**Thu 09**	**14:15-14:40**	**Room 3**

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IC144	Adelia Aquino	USA	Water-ionomer interfacial interactions investigated by infrared spectroscopy and computational methods.	**Thu 09**	**14:15-14:40**	**Room 4**
IC145	Jean-Sebastien Filhol	France	Including the electrochemical dimension into surface modelling and understanding.	**Thu 09**	**14:15-14:40**	**Room 5**
IC146	Jörg Grunenberg	Germany	Ill-defined concepts in computational chemistry: Quantum chemical bond orders.	**Thu 09**	**14:40-15:05**	**Room 1**
IC147	Raghavan B. Sunoj	India	Synergism between theory and experiments in asymmetric catalysis: transition state modelling for rationalizations and catalyst design.	**Thu 09**	**14:40-15:05**	**Room 2**
IC148	Anne-Clémence Corminboeuf	Switzerland	Quantification and analysis of intra- and intermolecular phenomena.	**Thu 09**	**14:40-15:05**	**Room 3**
IC149	Andreas Savin	France	Excitation energies along a range-separated adiabatic connection.	**Thu 09**	**14:40-15:05**	**Room 4**
IC150	Maria Joao Ramos	Portugal	Modelling enzymatic reactions.	**Thu 09**	**14:40-15:05**	**Room 5**
IC151	Sam B. Trickey	USA	Density functionals for systems under extreme conditions.	**Thu 09**	**15:05-15:30**	**Room 1**
IC152	C. David Sherrill	USA	Atomic- and fragment-partitioned symmetry-adapted perturbation theory for analyzing intermolecular interactions.	**Thu 09**	**15:05-15:30**	**Room 2**
IC153	Matthias Lein	New Zealand	Buckminsterfullerene adhesion on graphene flakes.	**Thu 09**	**15:05-15:30**	**Room 3**
IC154	Walter Thiel	Germany	Surface-hopping excited-states dynamics.	**Thu 09**	**15:05-15:30**	**Room 4**
IC155	Nigel Richards	USA	Energetics of C-C bond cleavage in oxalic acid and oxalate radicals: implications for the catalytic mechanism of oxalate decarboxylase.	**Thu 09**	**15:05-15:30**	**Room 5**
IC156	Yan Alexander Wang	Canada	The art of converging self-consistent-field calculations.	**Thu 09**	**15:30-15:55**	**Room 1**

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IC157	Alberto Vela	Mexico	Some applications of the electro donating and electro accepting powers to chemical reactivity.	**Thu 09**	**15:30-15:55**	**Room 2**
IC158	Odile Eisenstein	France	Non-classical CH; supramolecular interactions in control of diastereo selectivity.	**Thu 09**	**15:30-15:55**	**Room 3**
IC159	Donald G. Truhlar	USA	Electronically excited states, coupled potential energy surfaces, and photochemical dynamics.	**Thu 09**	**15:30-15:55**	**Room 4**
IC160	W. Andrzej Sokalski	Poland	Differential transition state stabilization as biocatalyst design tool.	**Thu 09**	**15:30-15:55**	**Room 5**
IC161	Wesley Allen	USA	Intramolecular dispersion.	**Thu 09**	**15:55-16:20**	**Room 1**
IC162	Oscar N. Ventura	Uruguay	Theoretical and experimental determination of the reactivity of HCC-CH2OH (2-propyn-1-ol) toward the OH radical at atmospheric conditions.	**Thu 09**	**15:55-16:20**	**Room 2**
IC163	Michael Filatov	Germany	Designing conical intersections for light-driven molecular machines: pure axial rotation is achieved in biomimetic molecular motors.	**Thu 09**	**15:55-16:20**	**Room 3**
IC164	Roman Curik	Czech Republic	Ab-initio calculations on resonant vibrational excitation of polyatomic molecules by electron impact.	**Thu 09**	**15:55-16:20**	**Room 4**
IC165	Yundong Wu	PR China	Development of residue-specific protein force fields.	**Thu 09**	**15:55-16:20**	**Room 5**
IC166	Angela Wilson	USA	Developments and modeling towards quantitative accuracy for the transition metals and beyond.	**Fri 10**	**10:30-10:55**	**Room 1**
IC167	Steven Wheeler	USA	Towards the rational design of organocatalysts for asymmetric propargylations of aromatic aldehydes.	**Fri 10**	**10:30-10:55**	**Room 2**
IC168	Dario Ariel Estrin	Argentina	QM/MM investigation of chemical reactivity of biomolecules.	**Fri 10**	**10:30-10:55**	**Room 3**

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IC169	Diego Venegas-Yazigi	Chile	Magnetic properties of molecular and extended inorganic systems: experiments and theory.	**Fri 10**	**10:30-10:55**	**Room 4**
IC170	Peter G. Szalay	Hungary	Building blocks of DNA and their excited state properties obtained by coupled-cluster methods.	**Fri 10**	**10:30-10:55**	**Room 5**
IC171	Pere Alemany Cahner	Spain	Analyzing the electronic structure of molecules using continuous symmetry measures.	**Fri 10**	**10:55-11:20**	**Room 1**
IC172	Richard M. W. Wong	Singapore	Catalytic activity and stereoselectivity of organocatalysts: interplay of noncovalent interactions.	**Fri 10**	**10:55-11:20**	**Room 2**
IC173	Fernando Gonzalez-Nilo	Chile	Structural analysis of the molecular self-assembly of amphiphilic dendrimer.	**Fri 10**	**10:55-11:20**	**Room 3**
IC174	Eliseo Ruiz	Spain	Mononuclear easy-plane single molecule magnets: a theoretical study.	**Fri 10**	**10:55-11:20**	**Room 4**
IC175	Stacey Wetmore	Canada	A computational study of DNA damage and repair.	**Fri 10**	**10:55-11:20**	**Room 5**
IC176	Shuhua Li	PR China	Electronic structure methods for large systems: recent developments and applications.	**Fri 10**	**11:20-11:45**	**Room 1**
IC177	Shengfa Ye	Germany	Mechanistic studies of O2 and CO2 activation by metalloenzymes and transtion metal complexes.	**Fri 10**	**11:20-11:45**	**Room 2**
IC178	Alfonso Hernández-Laguna	Spain	Ab-initio molecular dynamics study of the influence of octahedral charge in dehydroxylation reaction of 2:1 dioctahedral phyllosilicate models.	**Fri 10**	**11:20-11:45**	**Room 3**

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IC179	Chiara Cappelli	Italy	Towards a reliable modeling of chiroptical properties and spectroscopies.	**Fri 10**	**11:20-11:45**	**Room 4**
IC180	Renato Contreras	Chile	Molecular interactions in ionic liquids.	**Fri 10**	**11:20-11:45**	**Room 5**
IC181	Tom Ziegler	Canada	Constricted variational density functional theory. New developments.	**Fri 10**	**11:45-12:10**	**Room 1**
IC182	Chin Hui Yu	Taiwan	Tracking the reaction mechanism of organocatalysis.	**Fri 10**	**11:45-12:10**	**Room 2**
IC183	Wojciech Grochala	Poland	A different story of carbon.	**Fri 10**	**11:45-12:10**	**Room 3**
IC184	Dieter Cremer	USA	Novel tools to analyze chemical bonding and electronic structure based on vibrational spectroscopy: local vibrational modes.	**Fri 10**	**11:45-12:10**	**Room 4**
IC185	Kaline Coutinho	Brazil	Solvent effects on global reactivity properties for neutral and charged molecules using the sequential hybrid QM/MM method.	**Fri 10**	**11:45-12:10**	**Room 5**
IC186	Rodolfo Esquivel	Mexico	Quantum information-theoretical aspects of elementary chemical processes: concurrent processes and entanglement.	**Fri 10**	**13:25-13:50**	**Room 1**
IC187	Dong Hui Zhang	PR China	Theoretical studies of polyatomic reaction dynamics.	**Fri 10**	**13:25-13:50**	**Room 2**
IC188	Cherif F. Matta	Canada	The definition of electron localization-delocalization matrices (LDMS) and their use as an electronic fingerprinting tool in QSAR and molecular similarity modeling.	**Fri 10**	**13:25-13:50**	**Room 3**

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IC189	WanZhen Liang	PR China	Efficient approaches for the excited-state properties of molecules in vacuo and condensed media.	**Fri 10**	**13:25-13:50**	**Room 4**
IC190	Gerald Zapata-Torres	Chile	Seeking for Key Interactions to Understand Observed Activities in Monoamine Oxidase Ligands by Means of Transition State Structures	**Fri 10**	**13:25-13:50**	**Room 5**
IC191	Aldo H. Romero	USA	Structural search by the minima hopping method: theory and applications.	**Fri 10**	**13:50-14:15**	**Room 1**
IC192	Matthias Bickelhaupt	Netherlands	D regime, S regime and intrinsic bite-angle flexibility: new concepts for catalyst design.	**Fri 10**	**13:50-14:15**	**Room 2**
IC193	Rodrigo Capaz	Brazil	First-principles calculations of diameter and chirality dependences of optical and electronic properties of semiconducting single-wall carbon nanotubes.	**Fri 10**	**13:50-14:15**	**Room 3**
IC194	Masayoshi Nakano	Japan	Nonlinear optical properties of open-shell molecular systems: open-shell singlet molecules and molecular aggregates.	**Fri 10**	**13:50-14:15**	**Room 4**
IC196	O. Anatole von Lilienfeld	Switzerland	Alchemy and machine learning methods for the sampling of chemical space from first principles.	**Fri 10**	**14:15-14:40**	**Room 1**
IC198	Brian Yates	Australia	N2O reactivity with vanadium and n-heterocyclic carbenes.	**Fri 10**	**14:15-14:40**	**Room 3**
IC199	Alexandre Rocha	Brazil	Multiconfigurational approach to core-hole excited states.	**Fri 10**	**14:15-14:40**	**Room 4**

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ORAL PRESENTATIONS

OP code	Speaker	Country	Title	Day	Time	Room
OP001	Zhenhua Chen	P.R. China	Nonorthogonal orbital based N-body reduced density matrices and their applications to valence bond theory	**Mon 06**	**16:40-16:55**	**Room 1**
OP002	Jorge Martínez-Araya	Chile	Toward a prediction of catalytic activity, a pure experimental parameter, by means of local hyper-softness, a pure theoretical parameter	**Mon 06**	**16:40-16:55**	**Room 2**
OP003	Andrey Rogachev	US	Supramolecular aggregation of asymmetric n-heterocyclic carbenes: a theoretical insights into their unprecedented stability	**Mon 06**	**16:40-16:55**	**Room 3**
OP004	Luis Carlos Balbás	Spain	Structure, fragmentation patterns, and magnetic properties of small cobalt oxide clusters	**Mon 06**	**16:40-16:55**	**Room 4**
OP005	Joaquín Barroso	Mexico	Design of drug carriers through DFT calculations and molecular dynamics simulations: calix[n]arenes as hosts	**Mon 06**	**16:40-16:55**	**Room 5**
OP006	John Dobson	Australia	Ultra-long-ranged dispersion interaction between degenerate molecules	**Mon 06**	**16:55-17:10**	**Room 1**
OP007	Viktorya Aviyente	Turkey	A computational approach to the origins of stereoselectivity in organic reactions	**Mon 06**	**16:55-17:10**	**Room 2**
OP008	Georgi Vayssilov	Bulgaria	Computational studies of structure and properties of surface species on ceria	**Mon 06**	**16:55-17:10**	**Room 3**
OP009	Sergey I. Bokarev	Germany	Theoretical soft X-ray spectroscopy of transition metal compounds in solution	**Mon 06**	**16:55-17:10**	**Room 4**
OP010	Elena Laura Coitiño	Uruguay	New insights on the mechanism of biological thiols oxidation by H2O2: post-transition-state bifurcations in the reaction pathways	**Mon 06**	**16:55-17:10**	**Room 5**

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OP011	Martin Field	France	Advances in hybrid potential simulation of condensed phase systems	**Mon 06**	**17:10-17:25**	**Room 1**
OP012	Rosa Bulo	Netherlands	QM/MM simulations of aqueous systems	**Mon 06**	**17:10-17:25**	**Room 2**
OP013	Daniel Ess	US	Computational mechanisms and predictions of main-group-mediated alkane oxygen functionalization reactions	**Mon 06**	**17:10-17:25**	**Room 3**
OP014	Gloria Cárdenas-Jirón	Chile	Theoretical assessment of the photosensitization mechanisms of porphyrin-ruthenium(II) complexes for the formation of reactive oxygen species	**Mon 06**	**17:10-17:25**	**Room 4**
OP015	Fernando Cossío	Spain	Origins of the selectivity in the interaction between cisplatin and dna	**Mon 06**	**17:10-17:25**	**Room 5**
OP016	Graham Fletcher	US	The evaluation of wave functions constructed from overlapping orbitals for large-scale electronic structure applications	**Mon 06**	**17:25-17:40**	**Room 1**
OP017	Peeter Burk	Estonia	Computational study of lanthanide(III) aqua complexes	**Mon 06**	**17:25-17:40**	**Room 2**
OP018	Nicola Gaston	New Zealand	A balanced procedure for the treatment of cluster ligand interactions: gold clusters for catalysis	**Mon 06**	**17:25-17:40**	**Room 3**
OP019	Jeremy Coe	United Kingdom	Monte carlo configuration interaction: potential curves, transition metals and excited states	**Mon 06**	**17:25-17:40**	**Room 4**
OP020	Fernanda Duarte	Sweden	Understanding phosphoryl/sulfuryl transfer reactions: from model systems to enzymes	**Mon 06**	**17:25-17:40**	**Room 5**
OP021	Roberto Gomperts	US	Enabling gaussian on GPGPUS: progress report	**Mon 06**	**17:40-17:55**	**Room 1**

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OP022	Marco Caricato	US	Calculations of donor-acceptor electronic coupling for fret in gas phase and in solution: a comparison between coupled cluster and density functional theory	**Mon 06**	**17:40-17:55**	**Room 2**
OP023	Hannelore Goossens	Belgium	Triazolinediones enabling click and transclick reactions	**Mon 06**	**17:40-17:55**	**Room 3**
OP024	Ines Corral	Spain	Understanding how substitution alters the photophysical behavior of DNA/RNA nucleobases	**Mon 06**	**17:40-17:55**	**Room 4**
OP025	François Zielinski	United Kingdom	Calculation of raman optical activity spectra:a combined MD/DFT strategy for explicitly solvated carbohydrates	**Mon 06**	**17:40-17:55**	**Room 5**
OP026	Xiaosong Li	US	Low-scaling approximations to the equation of motion coupled-cluster singles and doubles equations	**Mon 06**	**17:55-18:10**	**Room 1**
OP027	David Danovich	Israel	Ab initio valence bond and block-localized wave function investigation of the nature of the halogen bond in the complexes of lewis bases with dihalogens	**Mon 06**	**17:55-18:10**	**Room 2**
OP028	R. Bruce King	US	Metal-metal multiple bonding: beyond the triple bond in metal carbonyls and cyclopentadienyls	**Mon 06**	**17:55-18:10**	**Room 3**
OP029	Ganglong Cui	P.R. China	Generalized trajectory surface-hopping method for internal conversion and intersystem crossing	**Mon 06**	**17:55-18:10**	**Room 4**

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OP030	Robert W. Góra	Poland	On the prebiotic route to nucleotides: solvent effects on the photochemistry of 2-aminooxazole and 4-aminoimidazole-5-carbonitrile	**Mon 06**	**17:55-18:10**	**Room 5**
OP031	Jorge Martin del Campo	Mexico	Self interaction error correction for hydrogen atom in GGA functionals	**Tue 07**	**16:40-16:55**	**Room 1**
OP032	Kelling J. Donald	US	The weak helps the strong: sigma holes and dative bonding	**Tue 07**	**16:40-16:55**	**Room 2**
OP033	László Túri	Hungary	Quantum dynamics of the isomers of water cluster anions: surface state vs. interior state clusters	**Tue 07**	**16:40-16:55**	**Room 3**
OP034	Claude Daul	Switzerland	Non-empirical prediction of the photophysical and magnetic properties of systems with open d- and f-shells based on LFDFT	**Tue 07**	**16:40-16:55**	**Room 4**
OP035	Petra Imhof	Germany	How DNA processing enzymes recognise their target site- insight from molecular simulations	**Tue 07**	**16:40-16:55**	**Room 5**
OP036	Lorenzo Maschio	Italy	Implementation of orbital-specific-virtuals for local electron correlation in periodic systems	**Tue 07**	**16:55-17:10**	**Room 1**
OP037	Tony Ford	South Africa	Structural, vibrational, energetic and electronic properties of the homodimers of the MH3X molecules (M=C,Si,Ge,Sn; X=F,Cl,Br,I)	**Tue 07**	**16:55-17:10**	**Room 2**
OP038	Juan Ignacio Rodriguez	Mexico	DFT/TDDFT study on the lowest energy isomers of the P3HT-PCBM dimer	**Tue 07**	**16:55-17:10**	**Room 3**
OP039	Martin Dracinsky	Czech Republic	The effects of fast molecular motions and nuclear delocalisation on nmr parameters	**Tue 07**	**16:55-17:10**	**Room 4**
OP040	Toyokazu Ishida	Japan	Probing protein environment in enzymatic processes: all-electron qm analysis combined with QM/MM modeling approach	**Tue 07**	**16:55-17:10**	**Room 5**

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OP041	Eduard Matito	Spain	New stringent conditions for the two-particle cumulant	**Tue 07**	**17:10-17:25**	**Room 1**
OP042	Tobias Kraemer	United Kingdom	Density functional study of a rhodium(I) sigma-alkane complex	**Tue 07**	**17:10-17:25**	**Room 2**
OP043	Georg Schreckenbach	Canada	Actinide–'pacman' complexes	**Tue 07**	**17:10-17:25**	**Room 3**
OP044	Daniel Henrik Friese	Norway	Multiphoton absorption calculation using an open-ended response theory approach - going beyond one- and two-photon absorption	**Tue 07**	**17:10-17:25**	**Room 4**
OP045	Tatyana Karabencheva-Christova	United Kingdom	Conformational dynamics of enzymes and enzyme-substrate complexes	**Tue 07**	**17:10-17:25**	**Room 5**
OP046	Monika Musial	Poland	The new coupled cluster method for the accurate description of a dissociation of the bond in alkali metal diatomics	**Tue 07**	**17:25-17:40**	**Room 1**
OP047	Paula Homem-de-Mello	Brazil	The driving force for methylene blue aggregation	**Tue 07**	**17:25-17:40**	**Room 2**
OP048	Pavel Stishenko	Russian Federation	Potential of lateral interactions of Co on Pt (111) fitted to recent STM images	**Tue 07**	**17:25-17:40**	**Room 3**
OP049	Stefan Knippenberg	Belgium	Non-linear optics simulations of cyanines	**Tue 07**	**17:25-17:40**	**Room 4**
OP050	Radek Marek	Czech Republic	Design of artificial dna quadruplexes for biological and nanomaterial applications	**Tue 07**	**17:25-17:40**	**Room 5**
OP051	Neil Ostlund	US	Semantic web portal for publishing results of computational chemistry	**Tue 07**	**17:40-17:55**	**Room 1**
OP052	Stephen Klippenstein	US	Striving for kinetic accuracy in a priori theoretical chemical kinetics	**Tue 07**	**17:40-17:55**	**Room 2**
OP053	Ole Swang	Norway	Computational determination of a mechanism for silicon island formation in sapo materials	**Tue 07**	**17:40-17:55**	**Room 3**

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OP054	Dmitry Makhov	United Kingdom	Ab initio multiple cloning algorithm for quantum nonadiabatic molecular dynamics	**Tue 07**	**17:40-17:55**	**Room 4**
OP055	Ricardo A. Matute	US	Origin of the fidelity of the DNA polymerase an EVP/FEP/US approach	**Tue 07**	**17:40-17:55**	**Room 5**
OP056	Konrad Patkowski	US	Basis set convergence of the post-CCSD(T) contribution to noncovalent interaction energies	**Tue 07**	**17:55-18:10**	**Room 1**
OP057	Rémi Maurice	France	The role of spin-orbit coupling on the chemical bonding in At2 and Ato+: analysis via effective bond orders	**Tue 07**	**17:55-18:10**	**Room 2**
OP058	Juan Torras	Spain	Experimental and theoretical study of silane deposition mechanism onto AA2024 alloy by means of organophosphonic acid	**Tue 07**	**17:55-18:10**	**Room 3**
OP059	Ricardo Mata	Germany	Unravelling the UV-vis absorption spectra of ThDP-dependent enzymes through QM/MM and incremental coupled cluster approaches	**Tue 07**	**17:55-18:10**	**Room 4**
OP060	Nelaine Mora-Diez	Canada	Deuterium isotope effects on acid-base equilibria	**Tue 07**	**17:55-18:10**	**Room 5**
OP061	Zilvinas Rinkevicius	Sweden	Quantum chemistry on a heterogeneous computer system: accelerating the kohn-sham method for hybrid CPU/GPGPU and CPU/INTEL mic platforms	**Thu 09**	**16:40-16:55**	**Room 1**
OP062	Junia Melin	US	Understanding thermal decomposition of double based propellants through quantum chemistry	**Thu 09**	**16:40-16:55**	**Room 2**
OP063	Jarkko Vähäkangas	Finland	Faraday rotation in graphene quantum dots: interplay between system size and perimeter type	**Thu 09**	**16:40-16:55**	**Room 3**

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OP064	John Parkhill	US	A role for dephasing in electronic structure theory	**Thu 09**	**16:40-16:55**	**Room 4**
OP065	Juan Jose Nogueira Perez	Australia	Enhancement of intersystem crossing by intercalation to dna	**Thu 09**	**16:40-16:55**	**Room 5**
OP066	Zoltán Rolik	Hungary	A quasiparticle-based multireference coupled-cluster method	**Thu 09**	**16:55-17:10**	**Room 1**
OP067	Renaldo Moura Jr.	Brazil	Chemical bond overlap properties in X3B–NH3 (X=F, Cl, Br) lewis adducts	**Thu 09**	**16:55-17:10**	**Room 2**
OP068	Dmitry Nerukh	United Kingdom	Hybrid molecular dynamics–hydrodynamics approach for multiscale modelling of liquid molecular systems	**Thu 09**	**16:55-17:10**	**Room 3**
OP069	Julien Pilme	France	The ELF and AIM topological analyses in the context of the quasirelativistic approach	**Thu 09**	**16:55-17:10**	**Room 4**
OP070	Jacek Korchowiec	Poland	Charge sensitivity analysis in the resolution of Force-Field atoms: formalism and applications	**Thu 09**	**16:55-17:10**	**Room 5**
OP071	Masanori Tachikawa	Japan	First-principles calculation for positron binding to molecules	**Thu 09**	**17:10-17:25**	**Room 1**
OP072	Ekaterina Pas	Australia	Importance of dispersion forces in ionic liquids: correlation with thermodynamic and transport properties	**Thu 09**	**17:10-17:25**	**Room 2**
OP073	Yi Zhao	P.R. China	Charge transfer in organic molecules for solar cells	**Thu 09**	**17:10-17:25**	**Room 3**
OP074	Hannes Raebiger	Brazil	Spin crossover of octahedral cobalt complexes	**Thu 09**	**17:10-17:25**	**Room 4**
OP075	Dmitry Osolodkin	Russian Federation	Molecular dynamics simulations of flavivirus envelope proteins	**Thu 09**	**17:10-17:25**	**Room 5**
OP076	Orlando Tapia Olivares	Sweden	A quantum multi-partite base framework for describing physico-bio-chemical processes	**Thu 09**	**17:25-17:40**	**Room 1**

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ORAL PRESENTATIONS

OP077	Tapio Rantala	Finland	Ab initio simulation of equilibrium chemical reactions	**Thu 09**	**17:25-17:40**	**Room 2**
OP078	Tarciso Andrade-Filho	Brazil	The role of confined water in peptide nanostructures	**Thu 09**	**17:25-17:40**	**Room 3**
OP079	Tulika Gupta	India	Quenching quantum tunneling of magnetization in lanthanide smms: a theoretical perspective	**Thu 09**	**17:25-17:40**	**Room 4**
OP080	Ulf Ryde	Sweden	Ligand-binding energies calculated with quantum-mechanical methods	**Thu 09**	**17:25-17:40**	**Room 5**
OP081	Victor Vysotskiy	Sweden	Adaptation of the molcas quantum chemistry package to modern hardware	**Thu 09**	**17:40-17:55**	**Room 1**
OP082	Pavlo Selyshchev	South Africa	Peculiarities of nonlinear chemical rate equations for kinetics of radiation defects accumulation	**Thu 09**	**17:40-17:55**	**Room 2**
OP083	Maria Cristina Menziani	Italy	A computational simulation of bio-corona formation on gold nanoparticles	**Thu 09**	**17:40-17:55**	**Room 3**
OP084	Dage Sundholm	Finland	Coupled-cluster and density functional theory studies of excited states of biochromophores	**Thu 09**	**17:40-17:55**	**Room 4**
OP085	Marc van Hemert	Netherlands	Molecular dynamics simulations of CO2 formation in interstellar ices	**Thu 09**	**17:40-17:55**	**Room 5**
OP086	Christof Walter	Germany	FF-sapt: physically-motivated intermolecular force fields from symmetry-adapted perturbation theory	**Thu 09**	**17:55-18:10**	**Room 1**
OP087	Avital Shurki	Israel	Insights on catalysis	**Thu 09**	**17:55-18:10**	**Room 2**
OP088	Akseli Mansikkamäki	Finland	Using density functional theory in the design of organic radical dimers with ferromagnetic interactions	**Thu 09**	**17:55-18:10**	**Room 3**

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ORAL PRESENTATIONS

OP089	Thorbjorn Juul Morsing	Denmark	A simple broken-symmetry DFT approach that quatitatively predicts the exchange coupling in dinuclear chromium(III) compounds	**Thu 09**	**17:55-18:10**	**Room 4**
OP090	Ross Walker	US	Fast and reliable ligand binding free energies - thermodynamic integration on GPUS	**Thu 09**	**17:55-18:10**	**Room 5**
OP091	Daniel Weber	Germany	Specialized potential energy surface investigations: capabilities of the cast program	**Fri 10**	**14:40-14:55**	**Room 1**
OP092	Clarissa Silva	Brazil	Specific rotation unveiling conformational and configurational equilibrium of pentoses in aqueous solution	**Fri 10**	**14:40-14:55**	**Room 2**
OP094	Alessandra Barbosa	Brazil	Shape resonances in low-energy-electron collisions with halopyrimidines	**Fri 10**	**14:40-14:55**	**Room 4**
OP095	Vivek Yadav	US	First principle molecular dynamics study of n methylacetamide in methanol	**Fri 10**	**14:40-14:55**	**Room 5**
OP096	Pawe Szarek	Poland	The relationship between size of an atom, its pearson hardness and its electronic polarizability	**Fri 10**	**14:55-15:10**	**Room 1**
OP097	Olga Stasyuk	Poland	Tautomerisation of thymine acts against the hückel 4n+2 rule: aromaticity and intermolecular interactions	**Fri 10**	**14:55-15:10**	**Room 2**
OP099	Corentin Boilleau	France	Redox modulation of luminescence	**Fri 10**	**14:55-15:10**	**Room 4**
OP100	Hsiao-Ching Yang	Taiwan	Exploring water dynamics the missing link for understanding enzyme structure and catalysis	**Fri 10**	**14:55-15:10**	**Room 5**
OP101	Thierry Leininger	France	The total position spread tensor in a molecular context	**Fri 10**	**15:10-15:25**	**Room 1**
OP102	Mark Waller	Germany	A density-based adaptive QM/MM method	**Fri 10**	**15:10-15:25**	**Room 2**

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ORAL PRESENTATIONS

OP104	Christo Christov	United Kingdom	Conformational flexibility, ligand binding, reaction mechanisms, and spectroscopic properties of enzymes	**Fri 10**	**15:10-15:25**	**Room 4**
OP105	Willian Novato	Brazil	Kinetics analysis for the ligand exchange reaction of his with a Pt(II) complex: an important step towards inactivating the beta-amyloid aggregates	**Fri 10**	**15:10-15:25**	**Room 5**
OP106	Jaroslaw Kalinowski	Finland	Reading the electronic wavefunction in molecular dynamics: isomerization and decomposition of a criegee intermediate in direct dynamics using a multireference potential	**Fri 10**	**15:25-15:40**	**Room 1**
OP109	Henryk Witek	Taiwan	Modeling infrared spectra of methanol clusters at finite temperature	**Fri 10**	**15:25-15:40**	**Room 4**

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POSTERS PRESENTATIONS

PP code	Presenting Author	Country	Title	Poster Sesion	Date
PP001	Carrión Samanta Magalí	Argentina	Testing the ability of various exchange-correlation functionals and basis set to describe properties of MO2, MO3, PT2 and PT3	**PS-1**	**Mon 06**
PP002	Ari Fernando Zeida	Argentina	Improving sampling efficiency in hybrid QM/MM simulations through a hybrid differential relaxation algorithm	**PS-1**	**Mon 06**
PP003	Stefan Vogt Geisse	Chile	Pydensity: an open source program for the computation of the dual descriptor for highly symmetric molecules	**PS-1**	**Mon 06**
PP004	Ofelia Oña	Argentina	Orbital localization procedure based on the topological analysis of the electron localization function	**PS-1**	**Mon 06**
PP005	Jason Rigby	Australia	New SCM- and SOS-MP2 coefficients fitted to semi-coulombic systems	**PS-1**	**Mon 06**
PP006	Bun Chan	Australia	Expanding the scope of wn-type protocols	**PS-1**	**Mon 06**
PP007	Gerd Rocha	Brazil	Accelerating semiempirical quantum chemical calculation by using multi-GPU platforms: implementations and benchmarks	**PS-1**	**Mon 06**
PP008	Renaldo Moura Jr.	Brazil	Chemical bond overlap properties in trans-1,2-disubstituted alkenes	**PS-1**	**Mon 06**
PP009	Ana Cristina Mora Tello	Brazil	Generation of gaussian basis set applying the polynomial generator coordinate method	**PS-1**	**Mon 06**
PP010	Itamar Borges Jr	Brazil	Molecular electronic structure and fragmentation via partition methods and nuclear Fukui functions	**PS-1**	**Mon 06**
PP011	Helen Nathalia Thompson	Brazil	Halogen bonding: a description by orbital interaction theory	**PS-1**	**Mon 06**
PP012	Regis Casimiro Leal	Brazil	Assessment of G3(MP2)//B3 theory with the original CEP-31G(d) basis set for molecules containing first- and second-row representative elements	**PS-1**	**Mon 06**
PP013	Cleuton De Souza	Brazil	Implementation of pseudopotential CEP in the G3X-MP3 and G3X(CCSD)-MP3 theories for assessing the enthalpy of formation	**PS-1**	**Mon 06**
PP014	Mauricio Gustavo Rodrigues	Brazil	Development of basis set from the GCM method using Q-exponentials	**PS-1**	**Mon 06**
PP015	Helio Dos Santos	Brazil	NLO-X (X=I-V): new gaussian basis sets for prediction of linear and nonlinear electric properties	**PS-1**	**Mon 06**
PP016	Diego Paschoal	Brazil	NMR-TZPP-DKH gaussian basis sets for NMR calculations - 195PT chemical shift	**PS-1**	**Mon 06**

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PP017	Felipe Fantuzzi	Brazil	Polar chemical bonds: a novel description from the quantum interference perspective	**PS-1**	**Mon 06**
PP018	Mauro Lúcio Franco	Brazil	All-electron double zeta basis sets for the most fifth-row atoms: application in DFT spectroscopic constant calculations	**PS-1**	**Mon 06**
PP019	Luiz Alberto Terrabuio	Brazil	Comparative investigation of charges and atomic dipoles from the partition based on Ehrenfest force fields	**PS-1**	**Mon 06**
PP020	Katharina Boguslawski	Canada	A multi-reference description of chemical systems with mean-field cost	**PS-1**	**Mon 06**
PP021	Matthew Chan	Canada	Efficient generation of two-electron integrals for geminal-based methods in HORTON	**PS-1**	**Mon 06**
PP022	Fernando Martin Boubeta	Argentina	Pka calculations using hybrid QM/MM schemes	**PS-1**	**Mon 06**
PP023	Toon Verstraelen	Belgium	An efficient protocol to derive reliable additive nonbonding force fields	**PS-1**	**Mon 06**
PP024	Michael S. Deleuze	Belgium	Quantum chemical and kinetic study of the oxidation mechanisms of naphthalene initiated by hydroxyl radicals. The H abstraction pathway	**PS-1**	**Mon 06**
PP025	Ana Paula de Lima Batista	Brazil	Theoretical insights into the silanol-assisted enamine formation in aldol reaction	**PS-1**	**Mon 06**
PP026	Jorge Soto-Delgado	Chile	A multiscale treatment for diels-alder reaction in solution; a QM/MM MD study	**PS-1**	**Mon 06**
PP027	Xin Xu	China	Fractional charge behaviour and band gap predictions with the XYG3 type of doubly hybrid density functionals	**PS-1**	**Mon 06**
PP028	Jonas Feldt	Germany	Development of a perturbative QM/MM Monte Carlo method for the study of molecules in solution	**PS-1**	**Mon 06**
PP029	Virineya Bertin Merdel	Mexico	Theoretical study of N2O reduction on Pt2 and Pt2O particles	**PS-1**	**Mon 06**
PP030	Nora Beatriz Okulik	Argentina	Study of intermediates in the acetilation of glycerol	**PS-1**	**Mon 06**
PP031	Andrea Claudia Bruttomesso	Argentina	Conformational and long-range anisotropy study of “V” shaped molecules: DFT calculations and NMR assignment of Tröger’s base diamide	**PS-1**	**Mon 06**
PP032	Margarita M. Vallejos	Argentina	Chemoselectivity and the regioselectivity of the reaction of dichloropropynylborane with 2-tert-butylbutadiene	**PS-1**	**Mon 06**
PP033	Walter Guerra	Argentina	Computational study of reactions of 2'-halo-[1,1'-biphenyl]-2-amines: synthesis of carbazoles by photostimulated intramolecular C–N coupling	**PS-1**	**Mon 06**

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PP034	Adriana Cecilia Olleta	Argentina	A theoretical study of and mechanisms in aprotic solvents: the role of intramolecular hydrogen bond nucleophiles	**PS-1**	**Mon 06**
PP035	Gustavo Aucar	Argentina	Electronic effects and the nature of intramolecular H-bond. A theoretical approach based on NMR spectroscopy	**PS-1**	**Mon 06**
PP036	Ari Fernando Zeida	Argentina	Understanding the catalytic ability of peroxiredoxins: a combined experimental and QM/MM study on the fast thiol oxidation step	**PS-1**	**Mon 06**
PP037	Nicolas Grimblat	Argentina	Theoretical investigation of the diels-alder reactions of pinacol alkenylboronates with cyclopentadiene	**PS-1**	**Mon 06**
PP038	María Fernanda Zalazar	Argentina	Study of confinement effects in H-beta and H-ZSM-5 zeolites by topological analysis of electron density	**PS-1**	**Mon 06**
PP039	Cecilia E. Silvana Alvaro	Argentina	Aromatic nucleophilic substitution in aprotic solvents: a theoretical study of 'dimer nucleophile mechanism'	**PS-1**	**Mon 06**
PP040	Darío J. R. Duarte	Argentina	Double lump-hole interaction between halogen atoms	**PS-1**	**Mon 06**
PP041	Steven Robert Kirk	China	AIMPAC2: a next-generation QTAIM code	**PS-1**	**Mon 06**
PP042	Rosana Maria Lobayan	Argentina	Exploratory conformational study of fenilflavan substituted with con R,R'=OH. Modeling of the polarizability and electric dipole moment	**PS-1**	**Mon 06**
PP043	Patricia Gabriela Belelli	Argentina	Density functional study of H2O dissociation on Au/alpha-Fe2O3: first step of water gas shift reaction	**PS-1**	**Mon 06**
PP044	Silvana Caglieri	Argentina	Theoretical study on amines structures	**PS-1**	**Mon 06**
PP045	Santiago Barrera Acevedo	Australia	Effect of basis sets, fundamental energetic components and counterpoise correction on Møller-Plesset opposite and parallel spin scaling coefficients in charge transfer (CT), S22 and S66 complexes	**PS-1**	**Mon 06**
PP046	Toon Verstraelen	Belgium	How to ensure the accuracy of polarizable force fields?	**PS-1**	**Mon 06**
PP047	Kristof De Wispelaere	Belgium	Molecular dynamics kinetic study on the zeolite-catalyzed methanol conversion	**PS-1**	**Mon 06**
PP048	An Ghysels	Belgium	Position-dependent diffusion profiles in inhomogeneous media	**PS-1**	**Mon 06**
PP049	Michael S. Deleuze	Belgium	Quantum chemical and kinetic study of the oxidation mechanisms of naphthalene initiated by hydroxyl radicals. I. The OH addition pathway	**PS-1**	**Mon 06**
PP050	Filippo Morini	Belgium	Exploring the electronic structure of biphenyl in momentum space	**PS-1**	**Mon 06**

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PP051	Pierre Olivier Hubin	Belgium	Modeling reactivity with a force field approach: the case of organocatalysis	**PS-1**	**Mon 06**
PP052	Sidney Ramos Santana	Brazil	Mechanisms of the thiophene hydrodesulfurization reactions employing a tungsten complex as catalyst	**PS-1**	**Mon 06**
PP053	Rafaela Costa	Brazil	Analysis of orbital population of pentacyclic triterpene with ursanic skeleton	**PS-1**	**Mon 06**
PP054	Gabriel Carvalho	Brazil	Assesment of semiempirical enthalpy of formation as scoring function to discriminate native structures in protein decoy sets	**PS-1**	**Mon 06**
PP055	Fernando Junior	Brazil	Absolute configuration of the biflavonoid agathisflavone determined by theoretical simulation of electronic circular dichroism spectra	**PS-1**	**Mon 06**
PP056	Victor Augusto Vianna Ferreira	Brazil	Electronic properties of 1,3-benzodioxole nucleus by localized molecular orbitals energy decomposition analysis (LMOEDA)	**PS-1**	**Mon 06**
PP057	Josene Maria Toldo	Brazil	Distortion/interaction and frontier molecular orbitals analysis in 1,3-dipolar cycloadditions: analysis of the selectivity of alkene-substituted with benzonitrile oxide	**PS-1**	**Mon 06**
PP058	Fernando Silva	Brazil	Born-oppenheimer molecular dynamics and electronic properties of pyridinium-iodide charge-transfer complexes in acetonitrile solution	**PS-1**	**Mon 06**
PP059	Orlando Roberto-Neto	Brazil	Trends in the energetic and bonding properties of neutral and charged magnesium clusters_N(N = 2 - 7) computed with the CCDT(T) and DFT methods	**PS-1**	**Mon 06**
PP060	Ayyaz Mahmood	Brazil	Quantum chemical investigation of selectivity and mechanism of gas-phase reactions: [R1R2CNO2]- + CH3I	**PS-1**	**Mon 06**
PP061	Égil Sá	Brazil	On activation step of hoveyda-grubbs catalyst	**PS-1**	**Mon 06**
PP062	Glauco Bauerfeldt	Brazil	Rate coefficient for the reaction of OH radical with (Z)-3-hexene - an experimental-theoretical study	**PS-1**	**Mon 06**
PP063	Patricia Perez	Chile	A computational and conceptual DFT study on the mechanism of hydrogen activation by frustrated lewis pairs	**PS-1**	**Mon 06**
PP064	Victor Lopes	Brazil	Theoretical calculations of rate coefficients for the OH addition reactions to C2 - C4 alkenes	**PS-1**	**Mon 06**
PP065	Gabriel Ernesto Jara	Brazil	Computational study of enzymatic phosphoryl-transfer reactions	**PS-1**	**Mon 06**
PP066	Pedro Augusto de Souza Bergamo	Brazil	Computational study of metal-azole complexes	**PS-1**	**Mon 06**

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PP067	Eder Henrique da Silva	Brazil	Theoretical study of aromaticity in squaraines	**PS-1**	**Mon 06**
PP068	Antonio Gustavo Sampaio de Oliveira-Filho	Brazil	Quasiclassical trajectory study of the OH + HBr --> H2O + Br reaction using a full-dimensional ab initio potential energy surface	**PS-1**	**Mon 06**
PP069	Desmond MacLeod Carey	Chile	Electronic structure of a diboraferrocene family	**PS-1**	**Mon 06**
PP070	Jorge Ignacio Martínez-Araya	Chile	Explaining reaction mechanisms using the dual descriptor: a complementary tool to the molecular electrostatic potential	**PS-1**	**Mon 06**
PP071	Vitor Hugo Menezes da Silva	Brazil	Theoretical study on regio- and stereoselective Heck-Matsuda arylation of allylic ester: a DFT-D3 approach	**PS-1**	**Mon 06**
PP072	Italo Anjos	Brazil	A DFT assessment of the noncovalent interactions in mesoionic dimers	**PS-1**	**Mon 06**
PP073	Lucas Fagundes Esteves	Brazil	Computational study of phosphate esters hydrolysis catalyzed by a model of catechol oxidase: catalytic promiscuity in biomimetic systems	**PS-1**	**Mon 06**
PP074	Heitor Avelino De Abreu	Brazil	Mechanism of cyanosilylation of aldehydes catalyzed by mil-101(CR)	**PS-1**	**Mon 06**
PP075	Rafael Piccoli	Brazil	Dimerization of cyclic trinuclear complexes: a structural insight	**PS-1**	**Mon 06**
PP076	Josefredo Pliego	Brazil	Mechanism of MeSPh oxidation by H2O2 inside an asymmetric confined Brønsted acid catalyst	**PS-1**	**Mon 06**
PP077	Thaciana Malaspina	Brazil	Quantifying the individual contribution of the hydroxyl groups to the free energy of hydration	**PS-1**	**Mon 06**
PP078	Fernanda Bettanin	Brazil	Dye-bilayer interaction: comparison between continuum and atomistic methods	**PS-1**	**Mon 06**
PP079	Edison Franco-Junior	Brazil	Development of a technique for analysis of diclofenac supported by density functional theory calculations	**PS-1**	**Mon 06**
PP080	Cleiton Maciel	Brazil	Aggregation of phenothiazine dyes in homogeneous and micro-heterogeneous media	**PS-1**	**Mon 06**
PP081	Kelson Mota T. Oliveira	Brazil	Stability and formation of clusters of lupane-type triterpenoids	**PS-1**	**Mon 06**
PP082	Carlos Cárdenas	Chile	How reliable is the Hard-Soft Acid-Base principle	**PS-1**	**Mon 06**
PP083	Sandro Marmitt	Brazil	Theoretical investigation of the reaction mechanism of carbon dioxide fixation catalyzed by 1-butyl-3-methyl-imidazolium bromide	**PS-1**	**Mon 06**
PP084	Ednilsom Orestes	Brazil	Insights into the interaction of CO2 with amines: a DFT benchmark study	**PS-1**	**Mon 06**
PP085	Joaquin Peralta	Chile	An integrated data driven reconstruction and molecular	**PS-1**	**Mon 06**

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			dynamics simulation for lattice structure in atom probe tomography		
PP086	Rodrigo Ormazabal-Toledo	Chile	A theoretical study of the mechanism of electro-cycloaddition between propylene oxide and CO2 catalyzed by [C4C1IM][Br]	**PS-1**	**Mon 06**
PP087	Norberto Jorge Castellani	Argentina	Structural and electronic properties of platinum doped titanium dioxide	**PS-1**	**Mon 06**
PP088	Patricia Gabriela Belelli	Argentina	Ammonia adsorption and dehydrogenation on fe nanoparticles	**PS-1**	**Mon 06**
PP089	Claudio Perez-Mendez	Chile	Unified model of nucleophilicity and electrophilicity. The interacting pair model.	**PS-1**	**Mon 06**
PP090	María Marta Branda	Argentina	Synthesis of methanol from CO hydrogenation on surfaces of ZnO (0001), CeO2(111) and ZnO/CeO2(111)	**PS-1**	**Mon 06**
PP091	Kerry Wrighton-Araneda	Chile	Keggin-type phosphopolyoxomolybdate - experimental and theoretical study	**PS-1**	**Mon 06**
PP092	Ricardo M. Ferullo	Argentina	Density functional study of Ag chemisorption on hematite	**PS-1**	**Mon 06**
PP093	Samuel Tan	Australia	Comparison of the effective fragment potential method with symmetry-adapted perturbation theory in the calculation of intermolecular interaction energies of ionic liquids	**PS-1**	**Mon 06**
PP094	Brad Wells	Australia	Charge equilibration methods for the efficient screening of metal-organic framework CO2 adsorbents	**PS-1**	**Mon 06**
PP095	Lennart Joos	Belgium	Computational study of the reversible opening and closing of the cok-14 zeolite	**PS-1**	**Mon 06**
PP096	Sebastián Gallardo Fuentes	Chile	Mechanistic insight into the ANRORC reaction of 1,4-dinitroimidazoles with aniline	**PS-1**	**Mon 06**
PP097	Quan Phung	Belgium	Atomic layer deposition of ruthenium: a theoretical insight	**PS-1**	**Mon 06**
PP098	Júlio Da Silva	Brazil	Dft calculations of epr parameters of anticancer ru(iii)/ru(ii) complexes	**PS-1**	**Mon 06**
PP099	Anderson Chaves	Brazil	Electronic properties and structural formation of binary pt-based clusters	**PS-1**	**Mon 06**
PP100	Rafael Freire	Brazil	Transition metals [Rh, Pd, Ir and Pt] adsorption on Cu(111) and Cu(111) surfaces: a theoretical investigation	**PS-1**	**Mon 06**
PP101	Samuel Silva	Brazil	Optical model for analysis of electromagnetic absorption of polymeric films loading with carbon black	**PS-1**	**Mon 06**
PP102	Lucas Andres Calderon	Colombia	Study of the catalytic role of nin clusters (n = 4, 6) in the h2-gasification of carbonaceous materials	**PS-1**	**Mon 06**

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PP103	Luiz Felipe Faria	Brazil	Structure of cyanate-anion ionic liquids: X-Ray scattering and simulations	**PS-1**	**Mon 06**
PP104	José Eduardo Padilha	Brazil	Directional control of the electronic and transport properties of graphynes	**PS-1**	**Mon 06**
PP105	Arthur Porto	Brazil	Exploring the potential energy surface for interaction of swcnt with NO2+	**PS-1**	**Mon 06**
PP106	Ricardo Vivas-Reyes	Colombia	Understanding the polar character trend in a series of Diels-Alder reactions using molecular quantum similarity and chemical reactivity descriptors	**PS-1**	**Mon 06**
PP107	Rogério Baierle	Brazil	Fe adsorption on the Si-terminated ;-SiC(001)-C(3x2) surface	**PS-1**	**Mon 06**
PP108	Ulises Javier JAUREGUI HAZA	Cuba	Interaction of paracetamol and 125i-paracetamol with surface groups of activated carbon: theoretical and experimental study	**PS-1**	**Mon 06**
PP109	Torres Antonio Felipe Cesar	Brazil	Electronic effects of different ligands and substituents on Zinc(II) porphyrins	**PS-1**	**Mon 06**
PP110	Luciano Costa	Brazil	Insights on the solubility of CO2 in 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide from the microscopic point of view	**PS-1**	**Mon 06**
PP111	Renato Pereira Orenha	Brazil	Ru-NO compounds: a computational study	**PS-1**	**Mon 06**
PP112	Juliana Mendes	Brazil	Evaluation of some organic molecules as potential corrosion inhibitors to (001) iron surface	**PS-1**	**Mon 06**
PP113	Bayron Cerda Rojas	Chile	Extraction and characterization of natural dyes for their use in dye sensitized solar cell	**PS-1**	**Mon 06**
PP114	Marta Ferraro	Argentina	Using anapole magnetizabilities for chiral discrimination	**PS-1**	**Mon 06**
PP115	Juho Roukala	Finland	Relativistic first principles analysis of the solid-state nuclear magnetic resonance data of novel 195pt complexes	**PS-1**	**Mon 06**
PP116	Nora Beatriz Okulik	Argentina	Computational study and spectroscopic investigations of the [Zn(Phen)2(CNGE)(H2O)](NO3)2•H2O complex	**PS-1**	**Mon 06**
PP117	Miguel Ponce-Vargas	Chile	A study on the versatility of metallacycles in host-guest chemistry: interactions in halide-centered hexanuclear copper (ii) pyrazolate complexes	**PS-1**	**Mon 06**
PP118	Ana Julieta Pepino	Argentina	Photoisomerization and thermal reversion of 5-arylmethylene-2-thioxoimidazolidin-4-one	**PS-1**	**Mon 06**

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PP119	Su Chen	Australia	Ab-initio prediction of proton NMR chemical shifts in imidazolium-based ionic liquids	**PS-1**	**Mon 06**
PP120	Stefan Knippenberg	Belgium	Simulating photochemistry: an investigation of excitonic coupling and photochromism effects	**PS-1**	**Mon 06**
PP121	Alvaro Muñoz-Castro	Chile	Axis-dependence of the magnetic response in fullerenes. Evaluation of the magnetic behavior of C36, C50, C60 and C70	**PS-1**	**Mon 06**
PP122	Roberto Haiduke	Brazil	A quadruple-zeta relativistic prolapse-free gaussian basis set: RPF-4Z	**PS-1**	**Mon 06**
PP123	Elmar Uhl	Brazil	The ionization spectra of nitromethane	**PS-1**	**Mon 06**
PP124	Silmar A do Monte	Brazil	Valence and rydberg states of CH3Cl: an MR-CISD study	**PS-1**	**Mon 06**
PP125	Rodrigo Lima	Brazil	Fano-rashba effect and enhancement of figure of merit in quantum dots	**PS-1**	**Mon 06**
PP126	Vinícius Manzoni	Brazil	Theoretical study of the solvent effect on nitrogen nmr shielding in azines	**PS-1**	**Mon 06**
PP127	Albano Carneiro	Brazil	Modeling 4F intensity parameters as a function of small distortions in LN(2,2'-bipyridine-1,1'-dioxide)4(ClO4)3 complexes (LN = PR3+ and ND3+)	**PS-1**	**Mon 06**
PP128	Daniel Cesar	Brazil	Effect of mn incorporation on the optical response of cdse quantum dot	**PS-1**	**Mon 06**
PP129	Carlos Eduardo Vieira de Moura	Brazil	Charge transfer dynamics of inner-shell states on PSIF-DBT films	**PS-1**	**Mon 06**
PP130	Hélcio Batista	Brazil	Investigation of the luminescence properties of polinuclear silacrown ether lanthanide complexes	**PS-1**	**Mon 06**
PP131	Pawel Tecmer	Canada	New geminal-based approaches in actinide chemistry	**PS-1**	**Mon 06**
PP132	Diego Cortés-Arriagada	Chile	Photophysical properties of Iridium (III) complexes to use in inter conversion energy devices	**PS-1**	**Mon 06**
PP133	German Barriga Gonzalez	Chile	Nitrone spin traps reactivity study using dual descriptor and SP-DFT Fukui Function	**PS-1**	**Mon 06**
PP134	Plinio Cantero López	Chile	The role of the MCP(CO)2 chromophore in the optical properties of the CPNTHMCP(CO)2 complexes, where M=Fe, Ru and Os; n=2 and 3	**PS-1**	**Mon 06**
PP135	Muhammad Shoaib	Arabia	Effect of reaction vessel pressure on the preparation of activated carbon from saudi date tree fronds (agro waste) by physical activation method	**PS-1**	**Mon 06**
PP136	Claudia Sandoval	Chile	Molecular simulation of inclusion complexes between flavonoids and amine-terminated pamam dendrimers	**PS-1**	**Mon 06**
PP137	Alexander Trujillo	Chile	Experimental and DFT study of allylic ferrocenyl chalcones: structure,	**PS-1**	**Mon 06**

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			spectroscopic and electrochemical properties.		
PP138	Elsayed Helmy	Egypt	A study of thermodynamic parameters of complexation of oxytetracycline hydrochloride (conductometric study)	**PS-1**	**Mon 06**
PP139	Kaido Tämm	Estonia	Theoretical modeling of HPV: QSAR and novodesign with fragment approach	**PS-1**	**Mon 06**
PP140	Aleksey Chumakov	Russia	Ab Initio calculations of DNA nucleobase pairs conduction confirm that adenine-thymine is isolator and guanine-cytosine is conductor	**PS-1**	**Mon 06**
PP141	Ricardo Soares	Brazil	Fumarate hydratase from leishmania major: the dimeric stability evaluated by molecular dynamics and protein crystallography	**PS-1**	**Mon 06**
PP142	Martin Magu	South africa	The development of a computer model for the determination of specific volatile & non-volatile organic pollutants present in south african water systems	**PS-1**	**Mon 06**
PP143	Nicolás Oscar Foglia	Argentina	No dependent reduction of Fe(III) heme proteins: insight from computer simulations	**PS-1**	**Mon 06**
PP144	Romina Brasca	Argentina	Derivatization reactions for fluorescence detection of anti-retroviral drugs. A DFT study	**PS-1**	**Mon 06**
PP145	Adriana B. Pierini	Argentina	Ledgins: relationship between conformational and inhibitory properties	**PS-1**	**Mon 06**
PP146	Jose Luis Borioni	Argentina	Derivatives of solanocapsine as inhibitors of acetylcholinesterase	**PS-1**	**Mon 06**
PP147	Gabriela Borosky	Argentina	In silico study on the catalytic mechanism of human placental alkaline phosphatase	**PS-1**	**Mon 06**
PP148	Andrés Mauricio Escorcia Cabrera	Colombia	Insights into the enantioselectivity of the candida antarctica lipase B catalyzed o-acetylation of (R,S)-propranolol - a QM/MM study	**PS-1**	**Mon 06**
PP149	Guillaume Fayet	France	Prediction of mixture properties based on QSPR models: the flash point of organic mixtures as a test case	**PS-1**	**Mon 06**
PP150	Emilio Angelina	Argentina	Topological analysis of the network of non-covalent interactions in halogen bonded biomolecular complexes	**PS-1**	**Mon 06**
PP151	Javier Eiras	Argentina	Molecular modelling studies of ketopiperazines steroidal mimetics as dual modulators on androgen receptor (AR) ;-hydroxylase/17,20liase (CYP17)	**PS-1**	**Mon 06**
PP152	María del Pilar Buteler	Argentina	Study of interactions between dendron behera amine and crystalline polypropylene surface	**PS-1**	**Mon 06**

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PP153	Robson da Silva Oliboni	Brazil	A QM/MM method for long range charge transfer	**PS-1**	**Mon 06**
PP154	Sebastián A. Andujar	Argentina	Theoretical study of the conformational behavior of small ligands in different environments	**PS-1**	**Mon 06**
PP155	Ana María Rodríguez	Argentina	Dynamic action mechanism of small antimicrobial	**PS-1**	**Mon 06**
PP156	Snezana Zaric	Qatar	Interactions of non-coordinated water and aqua complexes with water and benzene	**PS-1**	**Mon 06**
PP157	Yuji Naruse	Japan	Design of new axially-chiral 2,6-dichalcogenaspiro[3.3]heptane 2,6-dioxides: conformational fixation by the lone pair(s)	**PS-1**	**Mon 06**
PP158	Esteban Gabriel Vega Hissi	Argentina	Study of common base pair mismatches in DNA: a QTAIM analysis	**PS-1**	**Mon 06**
PP159	Nelida Maria Peruchena	Argentina	Small-size peptides acting as inhibitors of the bace1-exosite. A molecular modeling study using md simulations, qm calculations and qtaim analysis	**PS-1**	**Mon 06**
PP160	Alfonso Hernández-Laguna	Spain	Interaction of water on (001) basal surface of 2:1 dioctahedral phyllosilicates	**PS-1**	**Mon 06**
PP161	Gladis Laura Sosa	Argentina	Effect of molecular interactions between saccharides residues on stability of colloidal particles	**PS-1**	**Mon 06**
PP162	Aurora Costales	Spain	Can we calculate the thermodynamic properties of diamond and graphite?	**PS-1**	**Mon 06**
PP163	Lucas Joel Gutierrez	Argentina	Quantitative insight into the interactions between propargyl-linked antifolates and dihydrofolate reductase	**PS-1**	**Mon 06**
PP164	Lars Goerigk	Australia	The quantum-chemical treatment of peptides and proteins: are there better alternatives to the commonly used methods?	**PS-1**	**Mon 06**
PP165	Béla Fiser	Spain	Uranyl-glutathione interaction - a computational study	**PS-1**	**Mon 06**
PP166	Karmen Condic-Jurkic	Australia	P-glycoprotein transport fare: option flex	**PS-1**	**Mon 06**
PP167	Urban Bren	Austria	Pyranose dehydrogenase and neuraminidase promiscuity tackled by one-step perturbation and enhanced sampling techniques	**PS-1**	**Mon 06**
PP168	Thierry De Meyer	Belgium	Substituent effects on absorption spectra of ph indicators: an experimental and computational study of sulfonphthaleine dyes	**PS-1**	**Mon 06**
PP169	Margot Paulino	Uruguay	Assaying cyclosporin a and a set of analogues as inhibitors of a t.cruzi cyclophilin by docking and molecular dynamics	**PS-1**	**Mon 06**

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PP170	Vanesa Viviana Galassi	Brazil	Parametrization of an ubiquinone force field and simulation of membrane partition, diffusion and redox potentials	**PS-1**	**Mon 06**
PP171	Thereza A. Soares	Brazil	Polymorphism of lipopolysaccharide membranes: the effect of chemotypes, cations and temperature	**PS-1**	**Mon 06**
PP172	Alison Pacheco	Brazil	Structural analysis of aristololide and 9-ethoxyaristolactam iv – two secundary metabolities of phenantroid nature isolated of aristolochia argentina	**PS-1**	**Mon 06**
PP173	Ana Carolina Ferreira de Albuquerque	Brazil	Structure determination of sesquiterpenes by a parameterized protocol for NMR ^{13}C chemical shifts calculations	**PS-1**	**Mon 06**
PP174	Vanessa do Canto	Brazil	Interactions of monoamine oxidases a and b with neurotransmitters and 1,4-naphthoquinones ligands by docking and molecular dynamics simulations	**PS-1**	**Mon 06**
PP175	William Nitschke	Brazil	Structural study of jaburetox-v5 in POPC	**PS-1**	**Mon 06**
PP176	Eudes Fileti	Brazil	Molecular dynamics study of surfactant-like peptide based nanostructures	**PS-1**	**Mon 06**
PP177	Cristina Barboza	Brazil	Basis set and TD-DFT benchmark: singlet excited states of N,N'-bis(salicylidenes)	**PS-1**	**Mon 06**
PP178	TANIA SILVA	Brazil	Psychoactivity in cannabinoids compounds using cheminformatics	**PS-1**	**Mon 06**
PP179	Mateusz Brela	Poland	Olefin polymerization activity by electronic alternation on proximate of phenyl phenoxy ligand in half-metallocene titanium(iv) complexes	**PS-1**	**Mon 06**
PP180	Sandra Luber	Switzerland	New approaches for the calculation of local properties	**PS-1**	**Mon 06**
PP181	Liliana Mammino	South africa	Effects of the mutual positions of the two acyl groups in jensenone-precursored euglobals	**PS-1**	**Mon 06**
PP182	Weverson Gomes	Brazil	Molecular dynamics simulations of secondary structure stabilization of peptide by glicerol/water mixtures	**PS-1**	**Mon 06**
PP183	Valdemir Ludwig	Brazil	Molecular simulations on nanoconfined water molecules in finite-length armchair carbon nanotubes	**PS-1**	**Mon 06**
PP184	Rodrigo Gester	Brazil	Solvent effects on the lowest-lying n;* and;* excitations in derivatives of thieno[3,4-b]pyrazine	**PS-1**	**Mon 06**
PP185	Guilherme Menegon Arantes	Brazil	Fe-S bond stability in simple models and in mechanically stressed rubredoxin	**PS-1**	**Mon 06**

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PP186	Mauricio Angel Vega Teijido	Uruguay	Theoretical study of the inhibition mechanism of 1,2,4-thiadiazole derivatives in the cysteine protease cathepsin b (catb)	**PS-1**	**Mon 06**
PP187	Marcelo Andrade Chagas	Brazil	Solvent effects on the netal-to-ligand charge transfer transition of the complex [Ru(NH3)5(pyrazine)]2+	**PS-1**	**Mon 06**
PP188	Felippe Mariano Colombari	Brazil	Gamma-valerolactone force field development	**PS-1**	**Mon 06**
PP189	Guedmiller S. Oliveira	Brazil	Development of a computer-assisted nanobiosensor for pesticide monitoring	**PS-1**	**Mon 06**
PP190	Mauricio Coutinho-Neto	Brazil	Cu,Zn-sod redox energetics from a combination of dft and implicit solvent models	**PS-1**	**Mon 06**
PP191	Cristina Elizabeth Gonzalez Espinoza	Canada	Constrained-density functional theory tools for energy decomposition analyses	**PS-2**	**Tue 07**
PP192	Farnaz Heidar Zadeh	Canada	A new population analysis method that minimizes the information loss upon molecule formation	**PS-2**	**Tue 07**
PP193	Ofelia Oña	Argentina	A combined method of g-particle-hole hypervirial equation and equations-of-motion: a symmetry-adapted approach	**PS-2**	**Tue 07**
PP194	RAMIRO ARRATIA-PEREZ	Chile	Au62+: spin-orbit avoids further jahn-teller distortion, oh prevails!	**PS-2**	**Tue 07**
PP195	Carlos Cárdenas	Chile	Numerical exploration on the lieb-thirring bound	**PS-2**	**Tue 07**
PP196	Claudio Perez-Mendez	Chile	Electronic properties of elusive molecules in charged solvents.	**PS-2**	**Tue 07**
PP197	Rosana Maria Lobayan	Argentina	AIM/NBO conformational and stereoelectronic investigation of serotonin	**PS-2**	**Tue 07**
PP198	Steven Robert Kirk	China	The Pt site reactivity of the molecular graphs of Au6pt isomers	**PS-2**	**Tue 07**
PP199	James S. M. Anderson	China	The GKCI approach to truncating the FCI expansion for solving the electronic and nuclear schrödinger equation	**PS-2**	**Tue 07**
PP200	Julio Cesar Arce	Colombia	Marginal-condicional factorization of explicitly-correlated wavefunctions:s states of two-electron atoms	**PS-2**	**Tue 07**
PP201	Jhon Wilder Sánchez Obando	Colombia	Calculation of constitutional isomers and stereoisomers for: 1-chloro-2, 2-bis (trifluoromethyl) cyclopropane. Using polya's theorem enumeration	**PS-2**	**Tue 07**
PP202	Luca Guzzardi	Ecuador	Cut off in mathematical model to improve MRI	**PS-2**	**Tue 07**
PP203	Nadia Ben Amor	France	Towards linear scaling multireferential configuration interaction	**PS-2**	**Tue 07**

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PP204	Andreas Hansen	Germany	Performance of wave function based (local) correlation methods for the thermochemistry of large and difficult systems	**PS-2**	**Tue 07**
PP205	Marc Raupach	Germany	Periodic extension of the ETS-NOCV method -decomposition of the orbital relaxation term-	**PS-2**	**Tue 07**
PP206	Daniel Bellinger	Germany	Development of an algorithm for reaction path search: the implementation into the cast program	**PS-2**	**Tue 07**
PP207	Milica Andrejic	Germany	Hybrid QM/QM calculations on metal complexes - approaching the coupled cluster limit	**PS-2**	**Tue 07**
PP208	Kwangwoo Hong	Korea - republic of	Implementation of lagrange function-based density functional theory and its applications	**PS-2**	**Tue 07**
PP209	Renan Viesser	Brazil	Stereoelectronic effects on the 13C NMR deshielding of the iodobenzene derivatives	**PS-2**	**Tue 07**
PP210	Ronaldo Junior Fernandes	Brazil	Theoretical and experimental studies to elucidate the ring-opening metathesis polymerization mechanism performed by the [RuCl2(PPh3)2(piperidine)] catalyst	**PS-2**	**Tue 07**
PP211	Higo Cavalcanti	Brazil	Assessment of DFT methods on the prediction of the ground spin state of Mn(iii)t-4-pyp+, a superoxide dismutase mimics	**PS-2**	**Tue 07**
PP212	Rositca Nikolova	Bulgaria	Theoretical and experimental local reactivity parameters of 3-substituted coumarin derivatives	**PS-2**	**Tue 07**
PP213	Farnaz Heidar Zadeh	Canada	How reliable is the hard-soft acid-base (HSAB) principle?	**PS-2**	**Tue 07**
PP214	Nelaine Mora-Diez	Canada	Amide-imide tautomerism of acetohydroxamic acid in aqueous solution	**PS-2**	**Tue 07**
PP215	Stefan Vogt Geisse	Chile	Bonding, aromaticity, and planar tetracoordinated carbons in Si2CH2 and Ge2CH2	**PS-2**	**Tue 07**
PP216	Ana Paula de Lima Batista	Brazil	The Aza-Morita-Baylis-Hillman: a mechanistic insight on the conventional and bimolecular pathways	**PS-2**	**Tue 07**
PP217	Rocío Belén Durán	Chile	Reaction Force and Reaction Electronic Flux analysis of intramolecular proton transfers in DNA bases	**PS-2**	**Tue 07**
PP218	Daniela Guzmán Angel	Chile	Theoretical study of the proton transfer in formamide and the role of the water molecule in the reaction	**PS-2**	**Tue 07**
PP219	Ricardo Inostroza-Rivera	Chile	The mechanism of menshutkin reaction in gas and solvent phases from the perspective of the Reaction Electronic Flux	**PS-2**	**Tue 07**

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PP220	Daniela Ortega Ulloa	Chile	Study of the mechanism of carbocationic triple shift rearrangement	**PS-2**	**Tue 07**
PP221	Nery Andrés Villegas Escobar	Chile	The effect of substituents on the energy barrier in Diels-Alder reactions revisited	**PS-2**	**Tue 07**
PP222	katerine paredes	Chile	DFT study on the relative stabilities of substituted ruthenacyclobutane intermediates involved in olefin cross-metathesis reactions and their interconvertion pathways	**PS-2**	**Tue 07**
PP223	Glauco Bauerfeldt	Brazil	Reaction path and rate coefficients calculations for the reactions of OH radicals with the unsaturated alcohols: 2-methyl-2-propen-1-ol,3-buten-1-ol and 2-buten-1-ol	**PS-2**	**Tue 07**
PP224	Patricia Perez	Chile	A DFT analysis of the participation of zwitterionic TACs in polar [3+2] cycloaddition reactions	**PS-2**	**Tue 07**
PP225	Ricardo Pino Rios	Chile	Extending isomerization energy decomposition analysis to the study of chemical reactions. Case of study: the origin of the Alder-Stein endo rule	**PS-2**	**Tue 07**
PP226	Mario Saavedra	Chile	Interaction between dibenzyl disulfide and Cu(111)surface: a DFT study	**PS-2**	**Tue 07**
PP227	Eduardo Chamorro	Chile	Average local ionization potentials within the framework of the topological analysis of the electron localization function	**PS-2**	**Tue 07**
PP228	Rafael Islas	Chile	One substitution stops the B19(1-) wankel motor	**PS-2**	**Tue 07**
PP229	Carolina Olea	Chile	Theoretical study of the energy of interaction between cucurbit[7]uril and antineoplastic drugs cisplatin and oxaliplatin.	**PS-2**	**Tue 07**
PP230	Vitor Hugo Menezes da Silva	Brazil	DFT study for the regio-stereoselectivity formation of indanes mediated ring contraction of 1,2 dihydronaphthalenes by hypervalent iodine using microsolvated models	**PS-2**	**Tue 07**
PP231	Felipe Fantuzzi	Brazil	D2H versus D4H: origin of the molecular structure of cyclobutadiene from the generalized product function energy partitioning approach	**PS-2**	**Tue 07**
PP232	Jorge Ignacio Martínez-Araya	Chile	The dual descriptor and its possible use for a rational design of novel molecules with importance in nanoscience and nanotechnology	**PS-2**	**Tue 07**
PP233	Norberto Jorge Castellani	Argentina	Adsoption of al on graphene: DFT and MP2 calculations	**PS-2**	**Tue 07**
PP234	María Marta Branda	Argentina	Density functional theory study of NO2 dissociation on nanoparticles of Cu, Ag and Au	**PS-2**	**Tue 07**

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PP235	Rodrigo Ormazabal-Toledo	Chile	Effect of explicit water on imidazolium-based ionic liquids acidity and basicity	**PS-2**	**Tue 07**
PP236	Ricardo M. Ferullo	Argentina	Adsorption of small Au particles on goethite via density functional theory	**PS-2**	**Tue 07**
PP237	Pabla Barra	Chile	Free energy calculations of e-selectin-oligosaccharide interactions	**PS-2**	**Tue 07**
PP238	Karen Navarrete	Chile	Calculation of tubulin–epothilone binding free energy using thermodynamics integration method	**PS-2**	**Tue 07**
PP239	An Ghysels	Belgium	Diffusion through acidic zeolites with 8-membered rings	**PS-2**	**Tue 07**
PP240	Gloria Cardenas-Jiron	Chile	A computational chemistry study on the hydrolysis mechanism of ethyl acetate catalyzed by an aqueous molybdocene	**PS-2**	**Tue 07**
PP241	Eduardo Pacheco	Chile	Graphene supported hemin as an effective catalyst in oxidation reactions: a theoretical modelling	**PS-2**	**Tue 07**
PP242	Cristian Celis-Barros	Chile	Characterizing MAO-substrate transition state complexes by comparison of experimental kinetic data and quantum chemical cluster approach	**PS-2**	**Tue 07**
PP243	Silvia Diaz	Chile	HCN/CNH isomerization reaction assisted by water: an analysis based on the Reaction Electronic Flux and ETS-NOCV	**PS-2**	**Tue 07**
PP244	Moises Dominguez	Chile	Sequential QM/MM study of the spectral behavior of a solvatochromic bithiophene	**PS-2**	**Tue 07**
PP245	Sebastián Gallardo Fuentes	Chile	Is the pi stacking the responsible of the cation effect in the boulton-katritzky reaction?	**PS-2**	**Tue 07**
PP246	Égil Sá	Brazil	Solvatation of Hoveyda-Grubbs catalyst and olefin by water moistures	**PS-2**	**Tue 07**
PP247	Tao Fang	China	Investigating molecular crystals with periodic generalized energy-based fragmentation approach	**PS-2**	**Tue 07**
PP248	Lucas Andres Calderon	Colombia	Analysis of reaction profiles for early steps in a mechanism for H2-gasification of carbonaceous materials	**PS-2**	**Tue 07**
PP249	Rogério Baierle	Brazil	Electronic and structural properties of graphene, boron nitride and hybride c/bn nanoribbons nanoribbons.	**PS-2**	**Tue 07**
PP250	Ricardo Vivas-Reyes	Colombia	Quantum chemistry study of a series of 4-acetylamino-2-(3,5-dimethylpyrazol-1-yl)-6-pyridylpyrimidines: using quantum similarity descriptors	**PS-2**	**Tue 07**
PP251	Josefredo Pliego	Brazil	Prediction of phase equilibrium in binary liquid systems: combining the	**PS-2**	**Tue 07**

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			smd model with a modified regular solution theory		
PP252	Jorge Quintero-Saumeth	Colombia	Concerted double proton-transfer electron-transfer reaction between catechol or pyrogallol and superoxide radical anion	**PS-2**	**Tue 07**
PP253	Jasmina Sabolovic	Croatia	Density functional theory study for aqueous bis(l-histidinato)copper(ii) systems: validation of the B3LYP vs. MO6 results	**PS-2**	**Tue 07**
PP254	Ines Despotovic	Croatia	Metal cation complexes with tetrapyridine macrocyclic ligands - DFT calculations	**PS-2**	**Tue 07**
PP255	Gustavo Aucar	Argentina	Performance of different DFT functionals in full relativistic calculations of NMR properties	**PS-2**	**Tue 07**
PP256	Ulises Javier JAUREGUI HAZA	Cuba	Theoretical study of RE and TC DMSA complexes	**PS-2**	**Tue 07**
PP257	Ondrej Gutten	Czech republic	How simple is too simple? (computational perspective on importance of 2nd-Shell environment on Metal-ion binding)	**PS-2**	**Tue 07**
PP258	Cina Foroutan-Nejad	Czech republic	Incredible chemistry of stereo-electronically promoted super-lewis acids	**PS-2**	**Tue 07**
PP259	Zdenek Chval	Czech republic	Inverse hydration of the square planar platinum(ii) complexes: ab initio Molecular Dynamics study	**PS-2**	**Tue 07**
PP260	Patricia Rotureau	France	Theoretical approach to better understand industrial risks linked to the incompatibilities of ammonium nitrate	**PS-2**	**Tue 07**
PP261	Francois BAYARD	France	Multiscale analysis for crossing activation barriers, a possible way to a new nuclear reactor: the “ertigo” concept	**PS-2**	**Tue 07**
PP262	Rémi Maurice	France	The role of water molecules of the first solvation shell in modelling ligand-exchange reactions leading to ato+ hydrolyzed species	**PS-2**	**Tue 07**
PP263	Oleksandr Loboda	France	Geometry-dependent electric multipole and polarizability models for accurate ab initio water force fields	**PS-2**	**Tue 07**
PP264	Diego Marcelo Andrada	Germany	Bonding situation in a stable CSi3P five-membered cyclic cation	**PS-2**	**Tue 07**
PP265	Iris Antes	Germany	Calculation of protein-ligand binding affinities by QM/MM-based methods	**PS-2**	**Tue 07**
PP266	Jan Meisner	Germany	Kinetic isotope effects calculated with the instanton method	**PS-2**	**Tue 07**
PP267	Anna Heilos	Germany	Theoretical investigations on squaraine-based molecules	**PS-2**	**Tue 07**
PP268	Johannes Becker	Germany	Specialized investigations of organic compounds: the cast program in action	**PS-2**	**Tue 07**

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PP270	Melinda Krebsz	Hungary	Stability and dipolar cycloaddition reactions of Nitrile Selenides	**PS-2**	**Tue 07**
PP271	Tibor Pasinszki	Hungary	Theoretical study on the bis-indazolo-tetrachlororuthenate(iii) complex anion and its ferrocene analogue	**PS-2**	**Tue 07**
PP272	Sivakumar Radhakrishnan	Chile	Novel donor-acceptor ruthenium sensitizers for dye sensitized solar cells	**PS-2**	**Tue 07**
PP273	Alejandra Maureira	Chile	Theorical study of the energetic behavior on hydrogen activation reaction	**PS-2**	**Tue 07**
PP274	Diego Cortés-Arriagada	Chile	Adsorption of polycyclic aromatic pollutants on graphene	**PS-2**	**Tue 07**
PP275	César Barrales	Chile	1,3-dipolar cycloadditions: distortion/interaction model and Reaction Force analysis	**PS-2**	**Tue 07**
PP276	Walter Orellana	Chile	The physisorption of porphyrins on carbon nanotubes with full surface coverage: ab initio calculations	**PS-2**	**Tue 07**
PP277	Joaquin Peralta	Chile	Induced changes in surface bonding by electric field: integrating first principles and atom probe tomography	**PS-2**	**Tue 07**
PP278	Josene Maria Toldo	Brazil	TD-DFT study of benzazole derivatives: solvent effects and excited state intramolecular proton transfer mechanism(esipt)	**PS-2**	**Tue 07**
PP279	Miguel Ponce-Vargas	Chile	Host-guest interactions in di-halide mercuramacrocycle complexes	**PS-2**	**Tue 07**
PP280	Aleksey Chumakov	Russia	Ab initio calculations of DNA nucleotide bases transverse conduction confirm the feasibility of nucleobases identification by electrical current measurements	**PS-2**	**Tue 07**
PP281	Alvaro Muñoz-Castro	Chile	Sp3-hybridization in superatomic clusters. Analogues to simple molecules involving the Au6 core	**PS-2**	**Tue 07**
PP282	Andrés Aracena	Chile	Theoretical determination of properties in dithienylated and alkylated pyridinium salts	**PS-2**	**Tue 07**
PP283	Kerry Wrighton-Araneda	Chile	A theoretical electrochemical study of the mixed-valence dodecaalcoxo-hexavanadium cluster	**PS-2**	**Tue 07**
PP284	M. Leonor Contreras	Chile	Hydrogen physisorption energies for bumpy single walled nitrogen-containing carbon nanotubes	**PS-2**	**Tue 07**
PP285	Maria Luisa Ceron	Chile	Dual descriptor study in water gas shift reaction catalyzed by Cu supported on ZrO2	**PS-2**	**Tue 07**

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PP287	Cristian Oros	Chile	Computational design of graphene porphyrin based hybrid materials with photoelectronic applications	**PS-2**	**Tue 07**
PP288	Francisco Padilla	Chile	Theoretical modelling of cellulose-porphyrin complexes with antibacterial properties: characterization of the binding modes	**PS-2**	**Tue 07**
PP289	Fernando Mendizabal	Chile	Theoretical insights into the adsorption X-phenols (X= Se, Te) on gold (111)	**PS-2**	**Tue 07**
PP290	Tatiana Gómez	Chile	Influence of the TiO2 structural form (rutile and anatase surfaces vs. Cluster) on the sensitizer role of the dye	**PS-2**	**Tue 07**
PP291	Nancy Acelas	Colombia	Adsorption of phosphate and its competitive anions in wastewater onto Fe-(hydr)oxide: a molecular simulation	**PS-2**	**Tue 07**
PP292	Alejandro Morales Bayuelo	Colombia	Theoretical model for the polarization molecular and Hückel treatment of Phosphocyclopentadiene in an external electric field: hirschfeld study	**PS-2**	**Tue 07**
PP293	Anibal Alviz	Colombia	Ferrofluid flow in a channel induced by a rotating magnetic field	**PS-2**	**Tue 07**
PP294	Cina Foroutan-Nejad	Czech republic	Unveiling the unwilling bonding in U2C80: endohedral fullerene with a double 1e-2c u-u bonds	**PS-2**	**Tue 07**
PP295	Linda E. Robayo	Ecuador	Computational insights on montmorillonite surfaces modified with surfactants for environmental remediation applications	**PS-2**	**Tue 07**
PP296	Victor Posligua	Ecuador	Theoretical investigation of the potential of metal-functionalized pyrogallol[4]arenes as molecular hydrogen storage materials	**PS-2**	**Tue 07**
PP297	Patricio Puchaicela	Ecuador	Quantum-chemical modeling of doped SnO2	**PS-2**	**Tue 07**
PP298	Antti Karttunen	Finland	Semiconducting clathrates meet gas hydrates: Xe24[Sn136]	**PS-2**	**Tue 07**
PP299	Tapio Rantala	Finland	Ab initio correlated dynamics of electrons in 'artificial atoms'	**PS-2**	**Tue 07**
PP300	Diana Yepes	Chile	Photoemission spectra and density functional theory calculations of 3d transition metal-aqua complexes (Ti-Cu) in aqueous solution	**PS-2**	**Tue 07**
PP301	Walter Alfonso Rabanal León	Chile	A relativistic study of lanthanide hexa-azamacrocycles with aromatic lateral chains: electronic structure and optical properties	**PS-2**	**Tue 07**

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PP302	Desmond MacLeod Carey	Chile	Binuclear group vii carbonyls m2(CO)10 with m=mn, tc, re, bh. A relativistic theoretical study	**PS-2**	**Tue 07**
PP303	Ariel Rodrigo Guerrero	Chile	Raman and surface-enhanced raman scattering of 2-thio-5-nitrobenzoic acid with gold and silver nanoparticles: an experimental and theoretical study	**PS-2**	**Tue 07**
PP304	Natalia Hassan	Chile	Magneto-plasmonic nanopolymeric particles synthesized by microfluidic	**PS-2**	**Tue 07**
PP305	Natalia Inostroza	Chile	Rovibrational spectroscopic constants for isotopologues of cyclic and bent singlet HC2N isomers	**PS-2**	**Tue 07**
PP306	Karina Muñoz Becerra	Chile	A dft study of two polyoxovanadates containing the {V10O30} ring	**PS-2**	**Tue 07**
PP307	Martha Daza	Colombia	Internal heavy atom effects in phenothiazinium dyes: enhancement of intersystem crossing via vibronic spin-orbit coupling	**PS-2**	**Tue 07**
PP308	David Smith	Croatia	Calculating cd spectra for flexible biomolecules	**PS-2**	**Tue 07**
PP309	Radek Marek	Czech republic	Spin-orbit effects on the nmr chemical shifts in Ir(iii), Pt(ii), and Au(iii) complexes	**PS-2**	**Tue 07**
PP310	Liv Baerenholdt Klein	Denmark	Investigating excited state interactions in simple amines	**PS-2**	**Tue 07**
PP311	Thorbjorn Juul Morsing	Denmark	Calculating electronic and magnetic properties in transition metal complexes	**PS-2**	**Tue 07**
PP312	Kristian Baruël Ørnsø	Denmark	Optimizing porphyrins for dye sensitized solar cells using large-scale ab-initio calculations	**PS-2**	**Tue 07**
PP313	Siwar Chibani	France	TD-DFT simulation of the properties of the excited-states	**PS-2**	**Tue 07**
PP314	Matthew Kundrat	Germany	Modeling solvent effects on X-ray spectroscopy with frozen density embedding	**PS-2**	**Tue 07**
PP315	Deniz Tuna	Germany	Mechanisms of photostability in adenosine and glucose	**PS-2**	**Tue 07**
PP316	Charlotte Brueckner	Germany	Vb-based approaches to merocyanines with improved semiconducting properties	**PS-2**	**Tue 07**
PP317	Nickolas Charistos	Greece	Visualization of differences and similarities of the magnetic response of pi and sigma molecular orbitals in seven-membered boron wheels	**PS-2**	**Tue 07**
PP318	Mátyás Pápai	Hungary	Theoretical investigation of the light-induced spin transition in the [Fe(terpy)2]2+ complex	**PS-2**	**Tue 07**
PP319	MANU SIKARWAR	India	Ab initio calculation of the p-odd interaction constant wa in ybf using relativistic configuration-interaction approach	**PS-2**	**Tue 07**

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PP321	Kelson Mota T. Oliveira	Brazil	A configuration study of 17-o-metil akagerine, combining DFT calculations and NMR spectroscopy	**PS-2**	**Tue 07**
PP322	Guilherme Kilpp Gonzatti	Brazil	Glass formation of B-DNA hydration layer	**PS-2**	**Tue 07**
PP323	Wagner Richter	Brazil	Atomic ir intensities: relationship between effective charges and cssm model	**PS-2**	**Tue 07**
PP324	Mariana Batista	Brazil	Molecular movements and conformmational free energy profile PPAR-γ; helix 12	**PS-2**	**Tue 07**
PP325	Gabriela Borosky	Argentina	Mutagenic heteroaromatic amines: modelling the interactions with DNA	**PS-2**	**Tue 07**
PP326	Ricardo Soares	Brazil	Host phospholipid membrane bending capability of the dengue virus demonstrated by molecular dynamics simulations	**PS-2**	**Tue 07**
PP327	Alessandra Barbosa	Brazil	Low-energy electron scattering by cyclohexane	**PS-2**	**Tue 07**
PP328	Fábris Kossoski	Brazil	Potential energy surfaces for the anion states of 5-chlorouracil	**PS-2**	**Tue 07**
PP329	Corey MacDonald	Canada	The catalytic formation of leukotriene C4: a critical step in inflammatory processes	**PS-2**	**Tue 07**
PP330	Katie Wilson	Canada	A computational investigation of the replication of damaged DNA	**PS-2**	**Tue 07**
PP331	James Gauld	Canada	Multi-tasking as a way of enhancing 'specificity'? Pre-transfer editing in methionyl-trna synthetase	**PS-2**	**Tue 07**
PP332	David Sáez	Chile	Molecular dynamics simulations and force field parameterization of S-adenosylmethionine in the active site of catechol O-methyltransferase	**PS-2**	**Tue 07**
PP333	Sebastian E. Gutierrez-Maldonado	Chile	Characterizing the physicochemical properties of SiO2-supported membranes: a molecular dynamics study	**PS-2**	**Tue 07**
PP334	Carlos F. Lagos	Chile	Structure based virtual screening approaches for the identification of novel FXa inhibitors	**PS-2**	**Tue 07**
PP335	Raimundo Gillet	Chile	Molecular dynamics simulations of benzoic acid in water: relationship between interatomic distances and solubility	**PS-2**	**Tue 07**
PP336	Sebastián Esteban Miranda-Rojas	Chile	Towards an improved understanding of fluoroacetate dehalogenase reaction mechanism and selectivity	**PS-2**	**Tue 07**
PP337	Karel Mena Ulecia	Chile	Study of the affinity between the protein kinase pka and peptide substrates derived from kemptide by	**PS-2**	**Tue 07**

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			molecular dynamics simulations and MM/GBSA		
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PP339	Alejandro Vasquez-Espinal	Chile	Minimizing the risk of reporting false aromaticity and antiaromaticity in inorganic heterocycles following magnetic criteria	**PS-2**	**Tue 07**
PP340	Osvaldo Yañez-Osses	Chile	A classical molecular dynamics study on the role of residue N264 in the proton conductance through the voltage-gated proton channel hv	**PS-2**	**Tue 07**
PP341	Oscar Donoso	Chile	Traditional and ion-pair halogen bonds between chlorine and bromine derivatives and nitrogen-heterocyclic carbene	**PS-2**	**Tue 07**
PP342	Valeria Marquez	Chile	Dendrimer molecular design based on bioinformatics analysis of protein-DNA interactions	**PS-2**	**Tue 07**
PP343	Sandra Madariaga	Chile	Hydrogen bond between guanine and 2-naphtol: theoretical study at ab-initio level in gas phase and aqueous solution	**PS-2**	**Tue 07**
PP344	Eduardo Berríos	Chile	Human carbonic anhydrase ii: can a semi-empirical QM/MM model explain effects of active-site mutations over binding affinity	**PS-2**	**Tue 07**
PP345	Martin Floor	Chile	Design of a theozyme for the oxy-cope rearrangement	**PS-2**	**Tue 07**
PP346	Estefanía Hugo-Caselli	Chile	Role of Arg192 in the activity states of the D1 dopamine receptor	**PS-2**	**Tue 07**
PP347	Andy Mella	Chile	Study of properties of ionic liquid clusters using classical and ab-initio dynamics	**PS-2**	**Tue 07**
PP348	Montserrat Paola Peñaloza Amion	Chile	In the quest of important interactions between MAO and β-methyl phenethylamines: a steered molecular dynamic study	**PS-2**	**Tue 07**
PP349	Silvana Valdebenito	Chile	Characterization of inclusion complexes of beta-cyclodextrin with benzoxazinones derivatives: a theorical and experimental study	**PS-2**	**Tue 07**
PP350	Marcos Caroli Rezende	Chile	A comparison of the PCM/SDP continuum options for reproducing the negative solvatochromism of phenolate betaines	**PS-2**	**Tue 07**
PP351	Maximiliano Martínez-Cifuentes	Chile	A computational study of biologically active 2´-hydroxy chalcone derivatives	**PS-2**	**Tue 07**
PP352	Camila Muñoz	Chile	Study of binding affinity of novel a 2a agonists through computational methods	**PS-2**	**Tue 07**

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PP354	Cristian Celis-Barros	Chile	Triazolopiridine-cyclodextrin complex as aqueous metal chemosensor. A spectroscopy and theoretical study	**PS-2**	**Tue 07**
PP355	Carolina Mascayano	Chile	Steered molecular dynamic of selective inhibitors of 5- and 12-human lipoxygenase	**PS-2**	**Tue 07**
PP356	Rafael Gonzalez Hernandez	Colombia	Structural and electronical properties of si-doped gan non-polar surfaces	**PS-2**	**Tue 07**
PP357	Nelson David Arias Olivares	Colombia	Molecular dynamics analysis of human blood coagulation factor ix and its mutation A68T - G136V	**PS-2**	**Tue 07**
PP358	Pedro L. Acosta-Pérez	Colombia	Cgenff force field parameters for atenolol	**PS-2**	**Tue 07**
PP359	Daniel Iván Barrera	Colombia	Effect of mutations I189S and T138S on the population of near attack conformations during the o-acetylation of (R, S)-propranolol catalyzed by candida antarctica lipase B	**PS-2**	**Tue 07**
PP360	Markus Doerr	Colombia	Chemo- and enantioselectivity of candida antarctica lipase B catalyzing acetylation of (R,S)-propranolol - a combined docking and molecular dynamics investigation	**PS-2**	**Tue 07**
PP361	Daniel E. Trujillo González	Colombia	Bond characterization in first-row transition metal monoxide, dioxide, trioxide, peroxide, oxoperoxide, superoxide and oxosuperoxide	**PS-2**	**Tue 07**
PP362	Jorge Alfonso Charry	Colombia	Development and implementation of the explicitly correlated gaussian method in the any particle molecular orbital method	**PS-2**	**Tue 07**
PP363	Snezana Zaric	Qatar	Interactions of phenyl rings in proteins	**PS-2**	**Tue 07**
PP364	Andrés Mauricio Escorcia Cabrera	Colombia	Molecular modeling of the michaelis complexes in the acetylation of (R,S)-atenolol catalyzed by candida antarctica lipase S	**PS-2**	**Tue 07**
PP365	Sanja Tomic	Croatia	Multilevel computational study of human 3- hydroxyanthranilate 3,4-dioxygenase	**PS-2**	**Tue 07**
PP366	Martin Kabelá	Czech republic	Structure and dynamics of polypeptide proton wires in various environments	**PS-2**	**Tue 07**
PP367	Lorena Meneses	Ecuador	Computational infrared characterization of the synthesis of ibuprofen	**PS-2**	**Tue 07**
PP368	Kaido Tämm	Estonia	Predictive toxicology for regulatory affairs	**PS-2**	**Tue 07**
PP369	Fabienne BESSAC	France	Atomic scale simulation for the study of the interaction of pesticides with soil mineral matter.	**PS-2**	**Tue 07**

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PP372	Henry Chermette	France	Fragmentation mechanisms of DNA/RNA ionized bases	**PS-2**	**Tue 07**
PP373	Attila Kovács	Germany	Molecular properties of actinide trichlorides	**PS-2**	**Tue 07**
PP374	Natalia Kanaan Izquierdo	Germany	Quantum mechanical/ molecular mechanical studies in human thymine DNA glycosylase	**PS-2**	**Tue 07**
PP375	Deniz Tuna	Germany	Quantum-chemical investigations into the photophysics and photochemistry of bioorganic molecules	**PS-2**	**Tue 07**
PP376	Markus Hölscher	Germany	N2 activation and transformation to NH3 with H2 at diironthiolate catalysts supported by frustrated lewis pairs - a DFT study	**PS-2**	**Tue 07**
PP377	Ji Young Park	Korea - republic of	TCB 1: two-component based composite method	**PS-3**	**Thu 09**
PP378	Diego Moreno	Mexico	Kaxan, an global minimal search program	**PS-3**	**Thu 09**
PP379	Annia Galano	Mexico	Kinetics of radical molecule reactions in aqueous solution: a benchmark study on the performance of density functional methods	**PS-3**	**Thu 09**
PP380	Gabriel Moyocoyani Molina Espíritu	Mexico	Quantum entanglement and the 'spooky' chemical action at distance	**PS-3**	**Thu 09**
PP381	Simen Sommerfelt Reine	Norway	Improved auxiliary-density-matrix methods for the hartree-fock exchange contribution	**PS-3**	**Thu 09**
PP382	Tomasz Grining	Poland	Ultracold gas of fermions in a harmonic trap: a quantum chemical point of view	**PS-3**	**Thu 09**
PP383	Robert Moszynski	Poland	Asymptotic behavior of subradiant states in homonuclear diatomic molecules	**PS-3**	**Thu 09**
PP384	Aleksandra Tucholska	Poland	Transition moments between the excited electronic states from the hermitian formulation of the coupled cluster quadratic response function	**PS-3**	**Thu 09**
PP385	Carina Alicia Renison	South africa	Algorithms for GPU accelerated optimization & dynamics ab-initio modules	**PS-3**	**Thu 09**
PP386	Josep M. Oliva	Spain	A local spin procedure to determine heisenberg exchange coupling constants in clusters with magnetic sites	**PS-3**	**Thu 09**

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PP388	Aurora Costales	Spain	May IQA explain ionization potentials of small molecules?	**PS-3**	**Thu 09**
PP389	Eloy Ramos-Cordoba	Spain	Oxidation states from wavefunction analysis	**PS-3**	**Thu 09**
PP390	Juan Torras	Spain	An approach for multiple active zones in the hybrid QM/MM molecular dynamics methodology	**PS-3**	**Thu 09**
PP391	Evelio Francisco	Spain	A multipolar approach to the covalent interaction energy	**PS-3**	**Thu 09**
PP392	Jeremy Coe	United kingdom	Sum-over-states property calculations using Monte Carlo configuration interaction	**PS-3**	**Thu 09**
PP393	Ritchie Mae Gamot	United kingdom	Intelligent water drops algorithm with perturbation operators for atomic cluster optimization	**PS-3**	**Thu 09**
PP394	Piotr Piecuch	United states	Recent progress in the electron-attached, ionized, and active-space equation-of-motion coupled-cluster methodologies	**PS-3**	**Thu 09**
PP395	Luis Carlos Balbás	Spain	Theoretical study of ALNV+ clusters and their interaction with Ar	**PS-3**	**Thu 09**
PP396	Brandon Krull	United states	A non-empirical, fully non-local correlation functional free of self-interaction error based on a two-point correlation factor: implementation and preliminary results	**PS-3**	**Thu 09**
PP397	Haoyu Yu	United states	Exchange-correlation functional with broad accuracy, including single-multi-reference molecules and lattice constants	**PS-3**	**Thu 09**
PP398	Wenjing Zhang	United states	Tests of exchange-correlation functional approximations against reliable experimental data for average bond energies of 3d transition metal compounds	**PS-3**	**Thu 09**
PP399	Thomas Christian Jagau	United states	Complex absorbing potentials within eom-cc family of methods: theory, implementation, and benchmarks	**PS-3**	**Thu 09**
PP400	László Túri	Hungary	Quantized time correlation function approach to non-adiabatic decay rates in condensed phase	**PS-3**	**Thu 09**
PP401	Sreenithya Avadakkam	India	Mechanistic insights and origin of stereoselectivity in the excited state reaction of enone carboxamides: a density functional theory study	**PS-3**	**Thu 09**
PP402	Garima Jindal	India	Transition state models for probing cooperative asymmetric catalysis	**PS-3**	**Thu 09**
PP403	SAURABH KUMAR SINGH	India	Analyzing anisotropic exchange and double exchange in molecule based	**PS-3**	**Thu 09**

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			magnets using density functional calculations		
PP404	Faina Dubnikova	Israel	Quantum chemical calculations of the thermal decomposition of isoxazole and 5-methylisoxazole	**PS-3**	**Thu 09**
PP405	Vincenzo Aquilanti	Italy	Spin networks and quantum mechanical vector coupling: exact computation; hidden symmetries and semiclassical behavior of 3j symbols	**PS-3**	**Thu 09**
PP406	Lorenzo Maschio	Italy	The crystalline structure of folic acid	**PS-3**	**Thu 09**
PP407	Yuji Naruse	Japan	Conformational fixation by the lone pair(s): optical resolution of 2,6-dithiaspiro[3.3]heptane 2,6-dioxide	**PS-3**	**Thu 09**
PP408	Diego Cortés-Arriagada	Chile	Chemical interaction of hydrogen atom on graphene: insights from the reaction Force and Reaction Electronic Flux	**PS-3**	**Thu 09**
PP409	Shota Takamuku	Japan	Relationship between the open-shell characters and third-order nonliner optical properties of heteronuclear extended meatl atom chains	**PS-3**	**Thu 09**
PP410	David Samuel Rivera	Japan	A possible redox mechanism of the H2 interaction on BaTiO3(001)	**PS-3**	**Thu 09**
PP411	Yoshiaki Hayasaka	Japan	Computational calculations of multi-dimensional franck-condon factors in the analytical approach for 4-(dimethylamino) benzonitrile	**PS-3**	**Thu 09**
PP412	Akisumi Okamoto	Japan	Replica exchange md and ab initio fmo calculations for searching stable conformations of Amyloid-B (1-42) dimer and (9-42) dimer	**PS-3**	**Thu 09**
PP413	Kyung-Bin Cho	Korea - republic of	Does the rebound reaction really occur in nonheme metal-oxo systems?	**PS-3**	**Thu 09**
PP414	Lucia Pancoatl Moyotl	Mexico	Comparative theoretical study of inversion potential for NH3	**PS-3**	**Thu 09**
PP415	Nelly González-Rivas	Mexico	Chiral selective inclusion of sertraline estereoisomers in 2-hydroxypropyl-beta-cyclodextrin	**PS-3**	**Thu 09**
PP416	Joel Ireta	Mexico	Microsolvation as an approach to estimate the stability of solvated polyalanine in helical conformation	**PS-3**	**Thu 09**
PP417	Jesús Muñiz	Mexico	Modeling of transesterification process on triacetin using mgo model clusters as base heterogeneous catalysts for biodiesel production: a DFT study	**PS-3**	**Thu 09**
PP418	Marco Foscato	Norway	Automated design of organometallic compounds from fragments	**PS-3**	**Thu 09**
PP419	Rasmus Yding Brogaard	Norway	First principles modeling of solid acid catalysis supported by experiments: from kinetics to a reactivity descriptor	**PS-3**	**Thu 09**
PP420	Rafal Podeszwa	Poland	Predictions for water clusters from a first-principles two- and three-body force field	**PS-3**	**Thu 09**

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PP422	Wiktor Beker	Poland	Comparison of the enzyme-reactant stabilization a along reaction path with reaction force and reaction force constant	**PS-3**	**Thu 09**
PP423	Edward Brothers	Qatar	Density functional theory applied to reactions at metal centers	**PS-3**	**Thu 09**
PP424	Snezana Zaric	Qatar	Aromatic-aromatic interactions and nocovalent interactions of metal complexes	**PS-3**	**Thu 09**
PP425	Emilio Angelina	Argentina	From binding pocket to ligand structure	**PS-3**	**Thu 09**
PP426	Ana María Rodríguez	Argentina	New mimetic peptides inhibitors of a;-aggregation. Molecular guidance for rational drug design	**PS-3**	**Thu 09**
PP427	Vitaly Kiselev	Russian federation	Unexpected thermolysis reactions for insensetive energetic materials revealed by ab initio calculations	**PS-3**	**Thu 09**
PP428	Chiong Teck Wong	Singapore	Mechanisms of the alpha,alpha-diarylprolinol trimethylsilyl ether-catalyzed enantioselective reactions	**PS-3**	**Thu 09**
PP429	Antonija Lesar	Slovenia	HONO production from the reactions between organic peroxy radicals and NO	**PS-3**	**Thu 09**
PP430	Esteban Gabriel Vega Hissi	Argentina	Molecular insight into the interaction mechanism of amino-2H-imidazole derivatives with bace-1 protease: QM/MM investigations	**PS-3**	**Thu 09**
PP431	Alfonso Hernández-Laguna	Spain	Thermolysis reaction of 3,6-dimethyl-1,2,4,5-tetroxane	**PS-3**	**Thu 09**
PP432	AL Mokhtar Lamsabhi	Spain	Gas-phase interactions between lead(ii) ions and cytosine	**PS-3**	**Thu 09**
PP433	Oriana Brea Noriega	Spain	The total position spread tensor as a descriptor of the chemical bond	**PS-3**	**Thu 09**
PP434	José Pedro Cerón Carrasco	Spain	Proton transfer reactions in DNA: from spontaneous to induced genetic mutations	**PS-3**	**Thu 09**
PP435	Gladis Laura Sosa	Argentina	Dynamic and topology of protein/polyphenol molecular interactions	**PS-3**	**Thu 09**
PP436	Luis R. Domingo	Spain	A new reactivity model for C-C bond formation based on elf topologycal analisis of electron density	**PS-3**	**Thu 09**
PP437	Carmen Barrientos	Spain	Reactivity of alkaline-earth monocations with halomethane molecules: a computational kinetic study	**PS-3**	**Thu 09**
PP438	Xavier Solans-Monfort	Spain	DFT study on the reactivity of chelating ruthenium based alkene metathesis catalysts: effect of the ancillary ligands in their activity and z-/e- selectivity	**PS-3**	**Thu 09**

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PP440	Joakim Halldin Stenlid	Sweden	Mapping out unexplored areas of copper-water thermodynamics	**PS-3**	**Thu 09**
PP441	Beat Anton Amrein	Sweden	Force field independent metal parameters using a nonbonded dummy model	**PS-3**	**Thu 09**
PP442	Italo Andres Sanhueza	Switzerland	A case study on the success and failure of DFT methods to investigate metal catalyzed C-H functionalization reactions	**PS-3**	**Thu 09**
PP443	J. Samuel Arey	Switzerland	Intermolecular interactions of radicals and water	**PS-3**	**Thu 09**
PP444	Ito Chao	Taiwan	Are reliable DFT binding energies possible for large aromatic and aliphatic dimers?	**PS-3**	**Thu 09**
PP445	Hsiao-Ching Yang	Taiwan	Carbene rotamer switching controls the stereoselectivity of ring opening metathesis polymerization (romp) by ruthenium-catalysts	**PS-3**	**Thu 09**
PP446	Saron Catak	Turkey	Cinchona alkaloids as catalysts for the asymmetric ring-opening of meso-cyclic anhydrides	**PS-3**	**Thu 09**
PP447	Peter Repiscak	United kingdom	Computational modelling of complex copper systems: from cuno to copper macrocycles	**PS-3**	**Thu 09**
PP448	João Pedro Malhado	United kingdom	Comparing protonated schiff bases photoisomerization mechanisms in the gas phase	**PS-3**	**Thu 09**
PP449	Andrew Launder	United states	Computational elucidation of the CH3O2 + NO reaction pathways	**PS-3**	**Thu 09**
PP450	Andrey Rogachev	United states	Theoretical study of sandwich-like aggregates of buckybowls	**PS-3**	**Thu 09**
PP451	Giovanni Scalmani	United states	Domain decomposition approach for the effective application of implicit solvation models in qm/mm calculations	**PS-3**	**Thu 09**
PP452	Renat Sultanov	United states	Branching ratio in the O+HD->OH+D; OD+H reaction at low temperatures	**PS-3**	**Thu 09**
PP453	Steven Wheeler	United states	Anion-? Interactions with ?-acidic rings: it's not about the ?!	**PS-3**	**Thu 09**
PP454	Yaoming Xie	United states	Solvatation of hoveyda-grubbs catalyst and olefin by water moistures	**PS-3**	**Thu 09**
PP455	Ricardo A. Matute	United states	Nonstatistical dynamics of the triplet di-π-methane rearrangement	**PS-3**	**Thu 09**
PP456	Pragya Verma	United states	Mechanism of oxidation of C2H6 to C2H5OH on an iron-based metal-organic framework: a quantum mechanical study	**PS-3**	**Thu 09**

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PP458	Alicia Merlino	Uruguay	Stability and dynamics of VBC-HIF complexes under normoxic and hypoxic conditions	**PS-3**	**Thu 09**
PP459	Margot Paulino	Uruguay	Aspergillus nidulans dna-crea pattern recognition: in vitro and in silico studies	**PS-3**	**Thu 09**
PP460	Karmen Condic-Jurkic	Australia	Moderate structural response to radical chemistry: searching for an entrance into the active site for the second substrate during the two-step catalysis in pyruvate formate-lyase	**PS-3**	**Thu 09**
PP461	Jenner Bonanata	Uruguay	Modeling the reaction mechanism of sulfenic acid oxidation by hydrogen peroxide	**PS-3**	**Thu 09**
PP462	Gloria Buendia	Venezuela	A model for the catalytic oxidation of co that includes co desorption and diffusion, o repulsion and impurities	**PS-3**	**Thu 09**
PP463	Markus Hermann	Germany	Low coordinate germanium(ii) and tin(ii) compounds as catalysts for the hydroboration of carbonyl compounds	**PS-3**	**Thu 09**
PP464	Andreas Stegmueller	Germany	Growth processes in Gap/Si(001) semiconductor movpe: precursor decomposition mechanisms and surface effects	**PS-3**	**Thu 09**
PP465	Lucas Viani	Italy	On the correlations and exciton-phonon interactions in the PE545 light-harvesting complex	**PS-3**	**Thu 09**
PP466	Umpei Nagashima	Japan	Geometric isotope effects on small cloride ion water clusters	**PS-3**	**Thu 09**
PP467	Takayoshi Ishimoto	Japan	Theoretical study on interaction energy at graphene/water interface	**PS-3**	**Thu 09**
PP468	Noriyuki Kurita	Japan	Structures and electronic properties of metal organic frameworks: DFT and fmo calculations for model systems	**PS-3**	**Thu 09**
PP469	Yuichi Suzuki	Japan	Nanostructure of the aromatic polyamide membrane: apllication of hybrid MC/MD reaciton method	**PS-3**	**Thu 09**
PP470	Alejandro Bautista-Hernandez	Mexico	Stress-strain diagram of aluminum nanowires: tensile and compressive strain	**PS-3**	**Thu 09**
PP471	Hector Dominguez	Mexico	Adsorption of surfactant molecules on solid surfaces	**PS-3**	**Thu 09**
PP472	Juan Ignacio Rodriguez	Mexico	DFT/AM1 study on the structural and electronic properties of some electron donor polymers	**PS-3**	**Thu 09**
PP473	María Ivonne Baltazar Méndez	Mexico	Study and analysis of electronic and qtaim properties of Au4-S--Cn-H2n-S-Au4 complexes (n = 2-5)	**PS-3**	**Thu 09**

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PP475	Francesca Costanzo	Netherlands	Photo-oxidation of water on oxidic semi-conductor surfaces	**PS-3**	**Thu 09**
PP476	Nicola Gaston	New zealand	The superheating of gallium clusters explained? Observed phase transitions of the finite temperature polymorphs	**PS-3**	**Thu 09**
PP477	Kristof De Wispelaere	Belgium	Combined theoretical and experimental study on the influence of catalyst acid strength on the zeolite-catalyzed methanol conversion process	**PS-3**	**Thu 09**
PP478	Mateusz Brela	Poland	Theoretical analysis of ion-polymer interactions in pbi-based membranes with ets-nocv method	**PS-3**	**Thu 09**
PP479	Maria Natália Dias Soeiro Cordeiro	Portugal	Synthesis of nanoporous silica materials: from quantum mechanics to mesoscale modelling	**PS-3**	**Thu 09**
PP480	Alexandre Magalhaes	Portugal	Monte carlo study of phase transitions for model h2 confined in porous materials	**PS-3**	**Thu 09**
PP481	Matei-Maria Uta	Romania	Manganese-centered ten-vertex germanium clusters: in search of the missing link	**PS-3**	**Thu 09**
PP482	Nuno A. G. Bandeira	Spain	The essential role of dispersion effects in gold(i) catalysis: a case study	**PS-3**	**Thu 09**
PP483	Neyvis Almora-Barrios	Spain	Theoretical description of architectures of nanoparticles	**PS-3**	**Thu 09**
PP484	Saurabh Kumar Singh	India	Lanthanide based molecular magnets: origin of magnetic exchange and magnetic anisotropy in its details	**PS-3**	**Thu 09**
PP485	Enrique Gomez Bengoa	Spain	On the mechanism of the dynamic kinetic strategy for the asymmetric synthesis of chiral heterobiaryls	**PS-3**	**Thu 09**
PP486	Aleix Comas-Vives	Switzerland	Modeling supported metallic nanoparticles for the production of synthetic fuels	**PS-3**	**Thu 09**
PP487	Sandra Luber	Switzerland	Investigation of efficient catalysts for artificial water splitting	**PS-3**	**Thu 09**
PP488	Paul Day	United states	Linear and nonlinear optical properties of silver nanoclusters	**PS-3**	**Thu 09**
PP489	Kiet Nguyen	United states	Molecular metal chalcogenide clusters: a dft and tddft study	**PS-3**	**Thu 09**
PP490	Olexandr Isayev	United states	Materials cartography: representing and mining material space using structural and electronic fingerprints	**PS-3**	**Thu 09**
PP491	Lenin Díaz Soto	Venezuela	Theoretical study of the interaction of au+ and au4+2 cluster with mordenite	**PS-3**	**Thu 09**
PP492	Maria Cristina Menziani	Italy	Structural and optical properties of gold and silver nanoclusters	**PS-3**	**Thu 09**

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PP494	Yukichi Kitamura	Japan	Dual approach to vibrational spectra in solution: microscopic influence of hydrogen bonding to the state of motion of glycine in water	**PS-3**	**Thu 09**
PP495	oumkeltoum kabbaj	Marruecos	Dft study and spectroscopic analysis of the pesticide:imazerhapyr	**PS-3**	**Thu 09**
PP496	Daniel Henrik Friese	Norway	Optical rotation calculations on large molecules using the cc2 model and the resolution of the identity approximation	**PS-3**	**Thu 09**
PP497	Jean Pierre Inchaustegui	Peru	A dft study of the nonlinear optical properties of phthalocyanine derivatives	**PS-3**	**Thu 09**
PP498	Robert W. Góra	Poland	Estimation of excitation energy transfer couplings from distributed multipole moments	**PS-3**	**Thu 09**
PP499	Jozef Noga	Spain	Using of thouless expansion optimisation in scf procedure within the four-component relativistic scheme	**PS-3**	**Thu 09**
PP500	Carmen Lavín	Slovakia	Spectral properties of ch3 and sih3 radicals in the continuum region	**PS-3**	**Thu 09**
PP501	Claudia Climent	Spain	Solvatochromic effects on a donor-acceptor type organic dye with a quinoidal thiophene π-bridge	**PS-3**	**Thu 09**
PP502	Sebastian Keller	Switzerland	Excited state calculations with mps-dmrg	**PS-3**	**Thu 09**
PP503	Herbert Georg	Brazil	Solvent effect on the structural and electronic properties of molecules combining the sequential QM/MM and the free energy gradient methods	**PS-3**	**Thu 09**
PP504	Jhih-Wei Chu	Taiwan	Trajectory entropy of continuous stochastic processes at equilibrium	**PS-3**	**Thu 09**
PP505	Nuno Almeida	United kingdom	Challenging systems for quantum chemistry: intermolecular aggregates and inorganic excited states	**PS-3**	**Thu 09**
PP506	Morgane Vacher	United kingdom	Coupled electron-nuclear dynamics following photoionization of benzenes	**PS-3**	**Thu 09**
PP507	Michael Schmidt	United states	Valence virtual orbitals	**PS-3**	**Thu 09**
PP508	Megha Anand	United states	Non-innocent additives in a palladium catalyzed amination reaction	**PS-3**	**Thu 09**
PP509	Marco Caricato	United states	Theoretical simulations of uv/vis spectra for the screening of brown carbon compounds in atmospheric organic aerosol	**PS-3**	**Thu 09**
PP510	Rebecca Weber	United states	Structural and energetic properties for lanthanide systems	**PS-3**	**Thu 09**
PP511	Xiaosong Li	United states	Quantum coherent plasmon from the real-time tddft perspective	**PS-3**	**Thu 09**

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PP513	ANSTASIOS PAPADOPOULOS	Greece	Substituents' effects on pi electron delocalization in b-trisubstituted borazines based on visualization of molecular orbitals' contributions to the induced magnetic field	**PS-3**	**Thu 09**
PP514	Nidhi Vyas	India	Investigating the studies on the high-valent m-o(h)[m=fe and mn] complexes: a dft exploration	**PS-3**	**Thu 09**
PP515	Ashutosh Gupta	India	Exploring the mechanism of conversion of monosulfiram into disulfiram	**PS-3**	**Thu 09**
PP516	Avital Sharir-Ivry	Israel	Using valence bond (vb) to study catalysis and the effects of mutations in the haloalkane dehalogenase enzyme	**PS-3**	**Thu 09**
PP517	Daniele Narzi	Italy	Pathway for mn cluster oxidation by tyrosine-z in the s2 state of photosystem ii	**PS-3**	**Thu 09**
PP518	Daniele Bovi	Italy	Magnetic interactions in the mn_4cao_5 core of photosystem 2 by quantum mechanics/molecular mechanics simulations at room temperature	**PS-3**	**Thu 09**
PP519	Emanuele Coccia	Italy	Quantum monte carlo geometry optimization of chromophores of biological interest	**PS-3**	**Thu 09**
PP520	Masayoshi Takayanagi	Japan	Multiple oxygen entry pathways in t-state human hemoglobin revealed by intrinsic pathway identification method	**PS-3**	**Thu 09**
PP521	Hiroto Kikuchi	Japan	The loop opening motion of the bacterial xor with the inhibitor bof: molecular dynamics study	**PS-3**	**Thu 09**
PP522	yuki matsushita	Japan	Transcriptional mechanism controlled by lactose repressor protein and ligand elucidated by classical md and ab initio mo simulations	**PS-3**	**Thu 09**
PP523	Ernesto Chigo Anota	Mexico	Paracetamol adsorption on bn and bn oxide nanosheets	**PS-3**	**Thu 09**
PP524	Sandra Leticia Castillejos Mosqueda	Mexico	Theoretical study of ring opening polymerization mechanism of l-lactide and e-caprolactone with stannous 2-ethylhexanoate	**PS-3**	**Thu 09**
PP525	Said Jalife	Mexico	On the stability of ch62+	**PS-3**	**Thu 09**
PP526	Felipe Aparicio	Mexico	Dynamical properties and electronic effects in the protein – protein recognition process	**PS-3**	**Thu 09**

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PP529	Luis Mejia-Mazariegos	Mexico	Tautomerism in some pyrimidine nucleoside analogues used in the treatment cancer: from the point view of the electron density	**PS-3**	**Thu 09**
PP530	Romina Castañeda Arriaga	Mexico	Lipoic acid and dihydrolipoic acid. A comprehensive theoretical study of their antioxidant activity supported by available experimental kinetic data	**PS-3**	**Thu 09**
PP531	Myrna H. Matus	Mexico	Theoretical study of new derivatives of ferulic acid	**PS-3**	**Thu 09**
PP532	Rabaa Hassan	Morocco	Theoretical studies of a planar meso-substituted indolenine dibenzotetraaza[14]annulene ni(ii) complex	**PS-3**	**Thu 09**
PP533	Rosa Bulo	Netherlands	Multi-scale modeling of chemistry in water: applications in biomass conversion	**PS-3**	**Thu 09**
PP534	Nathaniel Gunby	New zealand	Molecular dynamics studies of flash evaporation of dilute solutions for chemical vapour deposition (cvd) processes	**PS-3**	**Thu 09**
PP535	Maria Luz Barreto Bermudez	Peru	Analysis of key structural properties for a study group of intermolecular parallel g-quadruplexes x-ray simulated with molecular dynamics	**PS-3**	**Thu 09**
PP536	Karol Dyduch	Poland	Theoretical studies on the cobalt(iii)-based catalysts for co2/epoxide copolymerization	**PS-3**	**Thu 09**
PP537	ROBERT ZALESNY	Poland	Solvent influence on vibrational first hyperpolarizability	**PS-3**	**Thu 09**
PP538	Alexandru Lupan	Romania	Metal-metal multiple surface bonding in polyhedral metallaborane clusters	**PS-3**	**Thu 09**
PP539	Kevin Alan Lobb	South africa	Determination of the mechanism of an unusual skeletal rearrangement of a spirobornyl tosylate derivative	**PS-3**	**Thu 09**
PP540	Ian Lloyd Rogers	South africa	Exploring enzymatic reactions with reaction dynamics and free energy surfaces	**PS-3**	**Thu 09**
PP541	Krishna Kuben Govender	South africa	Am1/d-cb1 and am1*-cb1: semi-empirical methods for qm/mm simulations of chemical glycobiology systems	**PS-3**	**Thu 09**
PP542	Poomany Penny Govender	South africa	Dft study of vitamin b12 analogues	**PS-3**	**Thu 09**
PP543	Zanele Precious Nhlabatsi	South africa	Computational study on the formation of glycine in the interstellar medium (ism)	**PS-3**	**Thu 09**

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PP545	Tancredo Fontineles	Brazil	Cryptolepine into DNA intercalation: a theoretical study using DFT electronic structure methods and molecular dynamics	**PS-3**	**Thu 09**
PP546	Werner Crous	South africa	Application of simple link atom saccharide hybrid (slash) methods to chemical glycobiological events	**PS-3**	**Thu 09**
PP547	María Fernanda Mendoza Muñoz	Spain	Molecular insights into synthesis of heparin/hs linker by retaining-glycosyltransferase extl2	**PS-3**	**Thu 09**
PP548	Sheila López-Rosa	Spain	Information-theoretic analysis of biological molecules	**PS-3**	**Thu 09**
PP549	Pilar Redondo	Spain	Formation of peptide bond in space through gas-phase reactions: formamide and acetamide	**PS-3**	**Thu 09**
PP550	Ferran Feixas	Spain	Accelerated molecular dynamics: a versatile tool to study protein folding and biomolecular recognition	**PS-3**	**Thu 09**
PP551	Jorge J. Carbo	Spain	Qsar methods for understanding and predicting the performance of organometallic catalysis	**PS-3**	**Thu 09**
PP552	Béla Fiser	Spain	Inhibitor design for trehalase proteins	**PS-3**	**Thu 09**
PP553	Klaudia Szeler	Sweden	Effects of high density lipoprotein (hdl) on the catalytic activity of paraoxonase-1 (pon1)	**PS-3**	**Thu 09**
PP554	Jiri Vanicek	Switzerland	On-the-fly ab initio semiclassical dynamics: emission spectra of oligothiophenes	**PS-3**	**Thu 09**
PP555	Bih-Yaw Jin	Taiwan	Nonlinear quantum transport in molecular junctions: a uniform theory bridging coherent tunneling and coulomb blockade limits based on the anderson's imputiy model	**PS-3**	**Thu 09**
PP556	Jen-Shiang K. Yu	Taiwan	Theoretical study of the dethiolation mechanism of human mercaptopyruvate sulfurtransferase upon cyanide removal	**PS-3**	**Thu 09**
PP557	Tsun-Tsao Huang	Taiwan	The stress introduced by mutations on a protein's active structure explains site-specific rates of evolution	**PS-3**	**Thu 09**
PP558	Rodrigo Cormanich	United kingdom	Elucidation of dipeptide model conformational preferences in solution by theoretical calculations and 1h nmr and infrared spectroscopies	**PS-3**	**Thu 09**
PP559	Pietro Aronica	United kingdom	Towards a new computational site-directed mutatgenesis protocol	**PS-3**	**Thu 09**
PP560	Sandor Lovas	United states	Development of peptide inhibitors of the human chaperone protein hsp70	**PS-3**	**Thu 09**

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PP562	Sameer Varma	United states	Allosteric regulation of nipah virus fusion with host cells	**PS-3**	**Thu 09**
PP563	Helen Nathalia Thompson	Brazil	Comparison between grf and spme methods in simulations of prion protein fragments	**PS-3**	**Thu 09**
PP564	Diego Carvalho	Uruguay	Quercetin target identification by reverse virtual screening	**PS-3**	**Thu 09**
PP565	Elena Maria Alvareda Migliaro	Uruguay	Antiinflamatory activity of phenolic compounds extracted from uruguayan propolis and grape (vitis vinifera) pomace: in vitro and in silico assays vinifera) pomace: in vitro and in silico assays	**PS-3**	**Thu 09**
PP566	Florencia Klein	Uruguay	In silico studies of histone h1's early glycation by ribose/adenosine diphosphate (adp) ribose and its synergy with protein oxidation	**PS-3**	**Thu 09**
PP567	Elena Laura Coitiño	Uruguay	Shedding light on the interaction mode of fatty acid nitroalkenes as agonists of the nuclear receptor pparg	**PS-3**	**Thu 09**
PP568	Stephanie Portillo	Uruguay	Unveiling the role of threonine44 in the catalytic mechanism of human peroxiredoxin 5	**PS-3**	**Thu 09**