WATOC 2017

11th Triennial Congress of the World Association of Theoretical and Computational Chemists

27 August – 1 September 2017
Munich, Germany

SCIENTIFIC PROGRAM

LMU LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN

www.watoc2017.com

Table of Contents

Words of Welcome

On behalf of the Local Scientific Committee, it is my pleasure to welcome you to the **11th Triennial Congress of the World Association of Theoretical and Computational Chemists** during the week of August 27 to September 1, 2017 in Munich, Germany. With about 1500 registered participants from all over the world and 12 plenary, 215 invited, 136 contributed speakers, as well as over 920 posters, WATOC2017 is the largest WATOC so far.

This shows both the increasing importance of theoretical and computational chemistry across the disciplines, and the central (and easy to reach) location of Munich in the heart of Europe. We have set up an exciting program covering a wide variety of cutting edge research topics ranging from method developments to applications pushing the limits of modern theoretical and computational chemistry, biochemistry, nanotechnology, and materials sciences.

WATOC2017 is held in the city center of Munich with both plenary and parallel sessions in the Gasteig cultural center under one roof. Besides great science, we hope that you will also find some time to explore the city of Munich and its surroundings which offer fascinating possibilities for both cultural and outdoor activities.

Even though I am sure that the many excellent lectures will make it difficult to decide which of the six parallel sessions to select, I hope you will enjoy WATOC2017 and your visit to Munich, both scientifically and culturally.

Christian Ochsenfeld , Chair of WATOC 2017

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WATOC

PROGRAM AT A GLANCE

Sunday, 27 August 2017

Time	Foyer
12:00 – 15:00	Registration

Time	Philharmonic Hall
15:00 – 15:50	Opening Ceremony
15:50 – 17:10	Plenary Session A Todd Martinez Benedetta Mennucci
17:10 – 17:40	Coffee Break
17:40 – 19:00	Plenary Session B Trygve Helgaker Helmut Schwarz

Time	Foyer
19:00 – 22:00	Welcome Reception – *supported by BASF*

Monday, 28 August 2017

Time	Philharmonic Hall	Carl-Orff Hall	Black Box	Small Concert Hall	Carl-Amery Hall	Multipurpose Room
09:00 – 09:40	Plenary Session C Edward Valeev					
09:40 – 10:10	Coffee Break					
10:10 – 12:15	Invited Session 1 Peter Gill Garnet Chan Jürgen Gauss Poul Jørgensen Martin Head-Gordon	Invited Session 2 Peter Schwerdtfeger Kwang Soo Kim Jean-Luc Bredas Marco Bernardi Jochen Blumberger	Invited Session 3 Lucas Visscher Neepa Maitra Sharon Hammes-Schiffer Eberhard Gross Katarzyna Pernal	Invited Session 4 Kenneth Ruud Pekka Pyykkö Wenjian Liu Trond Saue Marcel Swart	Invited Session 5 Hiromi Nakai Nuria Lopez Tore Brinck Stuart Macgregor Michelle Coote	Invited Session 6 Odile Eisenstein Michael Buehl Gustavo Aucar Ibon Alkorta Sotiris Xantheas
12:15 – 13:45	Lunch Break					
13:45 – 15:50	Invited Session 7 Jeremy Harvey Peter Richard Schreiner Leo Radom Yitzhak Apeloig Kendall Houk	Invited Session 8 Gustavo Scuseria Hans-Joachim Werner Örs Legeza Jeppe Olsen John Stanton	Invited Session 9 Weitao Yang Peter Pulay Henry F. Schaefer Dage Sundholm Petr Čársky	Invited Session 10 Kurt Kremer Florian Müller-Plathe Christoph Dellago Christine Peter Alexander Nemukhin	Invited Session 11 David Clary Irene Burghardt Roland Mitric Ivano Tavernelli Graham Worth	Invited Session 12 Benjamin Fingerhut Christel Marian Ilaria Ciofini Satoshi Maeda Henrik Koch
15:50 – 16:20	Coffee Break					
16:20 – 18:20	Contributed Session 1 Georg Schreckenbach Lorenzo Maschio Marek Sierka Joao B. L. Martins Wolfgang Hieringer Ralf Tonner Antti Karttunen Jon M. Matxain	Contributed Session 2 Thomas Kühne Tristan Bereau Ragnar Bjornsson Alister Page Olaf Wiest Dmitry Nerukh Laurence Leherte Xabier Lopez	Contributed Session 3 Shirin Faraji Oliver Kühn Debashree Ghosh Daniel Roca-Sanjuán Bo Durbeej László Turi Luca De Vico Valérie Brenner	Contributed Session 4 Manabu Sugimoto Tetsuya Taketsugu Mark Waller Seiji Mori Woo Youn Kim Anoop Ayyappan Wolfgang Quapp Michael Springborg	Contributed Session 5 Andreas Hauser Raul Alvarez-Idaboy Albeiro Restrepo Alessandro Contini Przemyslaw Dopieralski Joonkyung Jang Petra Imhof Wieslaw Nowak	Contributed Session 6 Mercedes Alonso Daniel Aravena Alexandre Magalhães Michal Straka Matthias Lein Juan F. Espinal Oscar Lung Wa Chung Amalia I. Poblador Bahamonde
18:20 – 20:00	Dinner Break					
20:00 – 22:00	Foyer Poster Session 1 – *supported by ACS Energy Letters*					

Tuesday, 29 August 2017

Time	Philharmonic Hall	Carl-Orff Hall	Black Box	Small Concert Hall	Carl-Amery Hall	Multipurpose Room
09:00 – 09:40	Plenary Session D Giulia Galli					
09:40 – 10:10	Coffee Break					
10:10 – 12:15	Invited Session 13 Walter Thiel Stefan Grimme Frank Jensen Siewert-Jan Marrink Jan H. Jensen	Invited Session 14 Ali Alavi Seiichiro Ten-no Roi Baer David Tannor Mark Gordon	Invited Session 15 Leticia González Roland Lindh Chantal Daniel George Schatz Joseph Subotnik	Invited Session 16 Joel Bowman Robert Berger R. Benny Gerber Lorenz S. Cederbaum Sergey Yurchenko	Invited Session 17 Fernando Martin Shaul Mukamel H. Bernhard Schlegel Peter Saalfrank Peter Knowles	Invited Session 18 Zexing Cao Tim Clark Markus Meuwly Sereina Riniker Xuhui Huang
12:15 – 13:45	Lunch Break					
13:45 – 15:50	Invited Session 19 Teresa Head-Gordon Jiali Gao Modesto Orozco Shina Caroline Lynn Kamerlin Helmut Grubmüller	Invited Session 20 Don Truhlar Carlo Adamo Kieron Burke G. Narahari Sastry David Sherrill	Industry Session 1 Peter Deglmann Christoph Taeschler Michael Edmund Beck Marcel Verdonk Thomas Fox	Invited Session 21 Michele Parrinello Ulf Ryde Zhipan Liu GuanHua Chen Michele Pavanello	Invited Session 22 Elfi Kraka Gabriel Merino Raghavan B. Sunoj Gopalan Rajaraman Laura Gagliardi	Invited Session 23 Takeshi Yanai Claudia Draxl Beate Paulus Krzysztof Szalewicz WanZhen Liang
15:50 – 16:20	Coffee Break					
16:20 – 18:20	Contributed Session 7 Mario Piris Heather Kulik Pierre-François Loos Henk Eshuis Jiri Klimes Eduard Matito Jan Řezáč Ekaterina Pas	Contributed Session 8 Andrey Rogachev Carsten Baldauf Brian Yates Hélène Bolvin Masato Kobayashi Lubomír Rulíšek Zahra Jamshidi Jean Christophe Tremblay	Industry Session 2 Glenn Jones Hanne Falsig Martin Letz Matthias Bremer Thomas Eckl	Contributed Session 9 Masayoshi Nakano Carmen Herrmann Takatoshi Fujita Paula Homem-de-Mello Tangui Le Bahers Basile F. E. Curchod William Glover Matthias Stein	Contributed Session 10 Mercè Deumal Nathalie Guihery Annika Bande Martin Rahm Ian Mackinnon Fernando Ruipérez Toyokazu Ishida Eliseo Ruiz	Contributed Session 11 Ferran Feixas Snezana Zaric Vladimir Palyulin José Pedro Cerón-Carrasco Niels Hansen Janos Daru Allan East Ole Swang
18:20 – 20:00	Dinner Break					
20:00 – 22:00	**Foyer** Poster Session 2 – *supported by The Journal of Physical Chemistry*					

Wednesday, 30 August 2017

Time	Philharmonic Hall	Carl-Orff Hall	Black Box	Small Concert Hall	Carl-Amery Hall	Multipurpose Room
09:00 – 09:40	Plenary Session E Pavel Hobza					
09:40 – 10:10	Coffee Break					
10:10 – 12:15	Invited Session 24 Alán Aspuru-Guzik Michele Ceriotti Markus Reiher Matthias Scheffler Gregory Voth	Invited Session 25 Sason Shaik Clémence Corminboeuf Julia Rice Matthias Bickelhaupt William Hase	Invited Session 26 Karsten Reuter Fabrizia Negri Mariachiara Pastore Biswarup Pathak Zhigang Shuai	Invited Session 27 David Tozer Hannes Jonsson Julien Toulouse Erin R. Johnson Matthias Ernzerhof	Invited Session 28 Marcus Elstner Elena Laura Coitiño Izaguirre Matthias Heyden Ville Kaila Holger Gohlke	Invited Session 29 Bogumil Jeziorski Manuel Yáñez Johannes Kästner Eluvathingal D. Jemmis Péter G. Szalay
12:15 – 13:00	Lunch Break					
13:00 – 20:00	Excursions					

20:00 – 22:00	**Löwenbräukeller** (Address: Nymphenburger Str. 2) Congress Dinner

Thursday, 31 August 2017

Time	Philharmonic Hall	Carl-Orff Hall	Black Box	Small Concert Hall	Carl-Amery Hall	Multipurpose Room
09:00 – 09:40	Plenary Session F Hiroshi Nakatsuji					
09:40 – 10:10	Coffee Break					
10:10 – 12:15	Invited Session 30 Filipp Furche Axel Becke Eunji Sim Andreas Görling Paul Ayers	Invited Session 31 Josef Michl Gernot Frenking Marco Nascimento Julia Contreras-García Russell J. Boyd	Invited Session 32 Chiara Cappelli Jacob Kongsted Lyudmila Slipchenko Fred Manby Kurt V. Mikkelsen	Invited Session 33 Anna Krylov Xiaosong Li Andreas Dreuw Spiridoula Matsika John Herbert	Invited Session 34 Rodney J. Bartlett Andreas Köhn Shuhua Li Jiri Pittner Ove Christiansen	Invited Session 35 Pedro Fernandes Yiqin Gao Young Min Rhee Carmay Lim David Smith
12:15 – 13:45	Lunch Break					
13:45 – 15:50	Invited Session 36 Richard Henchman Johan Åqvist Qiang Cui Pavel Jungwirth Gerhard Hummer	Invited Session 37 Marcel Nooijen Georg Kresse Silke Biermann Volker Blum Gregory Beran	Invited Session 38 So Hirata Dominika Zgid Denis Jacquemin Lucia Reining Wim Klopper	Invited Session 39 Toru Shiozaki David Tew Yuki Kurashige Hans Jørgen Aagaard Jensen Piotr Piecuch	Invited Session 40 Patrick Norman Daniel Crawford Benoît Champagne Sonia Coriani Antonio Rizzo	Invited Session 41 Igor Alabugin Miroslav Urban Attila Császár Annia Galano Munir Skaf
15:50 – 16:20	Coffee Break					
16:20 – 18:20	Contributed Session 12 Jan M.L. Martin Ricardo Mata Peter Nagy Graham Fletcher Jean-Philip Piquemal Joonsuk Huh Luca Frediani Sebastian Höfener	Contributed Session 13 Nick Mayhall Remco Havenith Andrzej L Sobolewski Thomas Koerzdoerfer Emanuele Coccia Robert Góra Isabelle Navizet Stefan Knippenberg	Contributed Session 14 Stella Stopkowicz Sandra Luber Malgorzata Biczysko Takeshi Iwasa Franco Egidi Sergei Ivanov Stepan Sklenak Alfonso Hernández-Laguna	Contributed Session 15 Martin Kaupp Lars Goerigk Sergei Vyboishchikov Arindam Chakraborty István Mayer Fan Wang Mikael P. Johansson Ran Friedman	Contributed Session 16 Mark Iron Sílvia Simon Ulrike Salzner Hong-Xing Zhang Martial Boggio-Pasqua Aurélie Perrier David Henry Thibaud Étienne	Contributed Session 17 José Enrique Barquera-Lozada Fabio Pichierri András Stirling Leonardo Belpassi Apostolos Kalemos David Wilson Ignacy Cukrowski Hugo Gattuso
18:20 – 20:00	Dinner Break					
20:00 – 22:00	**Foyer** Poster Session 3 – *supported by ACS Publications*					

Friday, 1 September 2017

Time	Philharmonic Hall
09:00 – 10:20	Plenary Session G Francesco Evangelista Johannes Neugebauer
10:20 – 10:50	Coffee Break
10:50 – 12:10	Plenary Session H Ursula Roethlisberger Frank Neese
12:10 – 12:50	Closing Ceremony and Poster Awards

SCIENTIFIC PROGRAM

Time	Foyer
12:00 – 15:00	REGISTRATION

Time	Philharmonic Hall	
15:00 – 15:50	**OPENING CEREMONY** *Chair: Christian Ochsenfeld* **Opening Schedule:** *Christian Ochsenfeld* (Chair of WATOC2017) *Walter Thiel* (WATOC President) *Barbara Conradt* (Vice President of the University of Munich (LMU)) *Helmut Schwarz* (President of Humboldt Foundation (AvH)) Music Intermezzo by *Ville Kaila (violin), Lika Bibileishvili (piano)*	
15:50 – 17:10	Plenary Session A *Chair: Peter Gill*	
15:50 – 16:30	**PL-1**	*Todd Martinez* Ground and excited state dynamics on graphical processing units
16:30 – 17:10	**PL-2**	*Benedetta Mennucci* Present and future of multiscale approaches combining quantum chemistry and classical models: a personal overview
17:10 – 17:40	COFFEE BREAK	
17:40 – 19:00	Plenary Session B *Chair: Leo Radom*	
17:40 – 18:20	**PL-3**	*Trygve Helgaker* Quantum chemistry in magnetic fields
18:20 – 19:00	**PL-4**	*Helmut Schwarz* Mechanistic variants of metal-oxide mediated C-H bond activation: experiment and theory in concert

Time	Foyer
19:00 – 22:00	**WELCOME RECEPTION** – *supported by BASF*

Time	Philharmonic Hall	Carl-Orff Hall	Black Box	Small Concert Hall	Carl-Amery Hall	Multipurpose Room
09:00 – 09:40	**PL-5** Plenary Session C *Chair: Kenneth Ruud* Edward Valeev Reduced scaling and controlled precision: extending the reach of many-body electronic structure					
09:40 – 10:10	COFFEE BREAK					
10:10 – 12:15	Invited Session 1 *Chair: Thomas Jagau*	Invited Session 2 *Chair: Tim Clark*	Invited Session 3 *Chair: Tomasz Wesolowski*	Invited Session 4 *Chair: Hans Jørgen Aagaard Jensen*	Invited Session 5 *Chair: Manabu Sugimoto*	Invited Session 6 *Chair: Henry Rzepa*
10:10	**I-011** *Peter Gill* Strong correlation in electron gases	**I-021** Peter Schwerdtfeger From graphene to graphyne, fullerenes, fulleroids, gaudienes and their golden duals	**I-031** Lucas Visscher Subsystem and approximate DFT approaches for electronically excited states of complex molecular systems	**I-041** Kenneth Ruud 4-component relativistic calculations with periodic boundary conditions	**I-051** *Hiromi Nakai* Chemical reaction simulations on CO2 chemical absorption process	**I-061** *Odile Eisenstein* Can carbon-13 NMR chemical shifts inform on reactivity in organometallic chemistry?
10:35	**I-012** *Garnet Chan* Notes on the complexity of electronic structure theory	**I-022** Kwang Soo Kim Graphene nanoribbon based electronics and spintronics	**I-032** Neepa Maitra Confronting memory-dependence in time-dependent density functional theory	**I-042** *Pekka Pyykkö* Recent results on compounds of heavy, and heaviest elements	**I-052** *Nuria Lopez* New aspects in the simulations of heterogeneous catalysis	**I-062** *Michael Buehl* Exploring NMR properties of paramagnetic Cu phenolic oxime complexes
11:00	**I-013** *Jürgen Gauss* Beyond standard coupled-cluster theory and towards full configuration interaction	**I-023** Jean-Luc Bredas Polymer/fullerene solar cells: characterization of the intermolecular interactions and interfacial charge-transfer states	**I-033** Sharon Hammes-Schiffer Multicomponent density functional theory: integrating electronic and nuclear quantum effects	**I-043** *Wenjian Liu* New Scenarios for Strongly Correlated Electrons	**I-053** *Tore Brinck* σ-hole Bonding in the Catalysis of Nanostructured Metals: Surface Properties as Guides to Local Reactivity	**I-063** *Gustavo Aucar* NMR spectroscopic paramaters of HB containing molecules and agregates of DNA base pairs
11:25	**I-014** *Poul Jørgensen* Cluster perturbation theory for energies and molecular properties	**I-024** Marco Bernardi Advances in computing charge carrier dynamics from first principles	**I-034** Eberhard Gross Potential-energy surfaces and Berry phases beyond the born-oppenheimer approximation: a new perspective on non-adiabatic dynamics	**I-044** *Trond Saue* Variational perturbation theory in geochemistry	**I-054** *Stuart Macgregor* Modelling alkane σ-Complexes in the solid state	**I-064** *Ibon Alkorta* Anion-anion and cation-cation halogen and hydrogen bonded complexes
11:50	**I-015** *Martin Head-Gordon* Some recent advances in variational energy decomposition analysis of electronic structure calculations	**I-025** Jochen Blumberger Simulation of electron transfer on the nanoscale: from molecules to biomolecules to materials	**I-035** Katarzyna Pernal Adiabatic connection approach toward including dynamic correlation for multireference wavefunctions	**I-045** *Marcel Swart* Characterization of reactive high-valent transition-metal complexes	**I-055** *Michelle Coote* Directionality and the role of polarization in electrostatic catalysis	**I-065** *Sotiris Xantheas* Modeling of the spectroscopic signatures of water in different environments
12:15 – 13:45	LUNCH BREAK					

Time	Philharmonic Hall		Carl-Orff Hall		Black Box		Small Concert Hall		Carl-Amery Hall		Multipurpose Room	
13:45 – 15:50	Invited Session 7 *Chair: Henrik Zipse*		Invited Session 8 *Chair: Martin Head-Gordon*		Invited Session 9 *Chair: Hiromi Nakai*		Invited Session 10 *Chair: H. Bernhard Schlegel*		Invited Session 11 *Chair: Oliver Kühn*		Invited Session 12 *Chair: Stefan Knippenberg*	
13:45	**I-071**	*Jeremy Harvey* Modelling reaction mechanisms and kinetics in homogeneous catalysis: challenges and progress	**I-081**	Gustavo Scuseria Symmetry projected coupled cluster theory	**I-091**	Weitao Yang Localized orbital scaling correction for systematic elimination of delocalization error in density functional approximations	**I-101**	*Kurt Kremer* Open systems simulations of macromolecular solutes through adaptive resolutions simulations (AdResS)	**I-111**	*David Clary* Quantum dynamical and semi-classical calculations on chemical reactions with application to decomposition of nerve agents	**I-121**	*Benjamin Fingerhut* Numerical exact MACGIC-QUAPI simulations of electron transfer dynamics in Drosophila cryptochrome (dCRY)
14:10	**I-072**	*Peter Richard Schreiner* London dispersion effects in molecular chemistry – reconsidering steric effects[1]	**I-082**	Hans-Joachim Werner Accurate treatment of long-range correlation effects in large molecules using explicitly correlated local coupled-cluster methods	**I-092**	Peter Pulay Ultrafast quantum/molecular mechanics: thermodynamic integration and van der Waals parameters	**I-102**	*Florian Müller-Plathe* Multiscale molecular modelling of soft materials: the challenge of dynamics	**I-112**	*Irene Burghardt* High-dimensional quantum dynamics of functional organic polymer materials: Coherence, localization, and (dis)order	**I-122**	*Christel Marian* TADF efficiencies in coinage-metal coordination complexes and metal-free donor-acceptor systems
14:35	**I-073**	*Leo Radom* Impact of hydrogen bonding on the susceptibility of peptides to oxidation	**I-083**	Örs Legeza Tensor product methods and entanglement measures for strongly correlated molecular systems	**I-093**	Henry F. Schaefer Fast construction of the exchange operator in an atom-centered basis with concentric atomic density fitting	**I-103**	*Christoph Dellago* Exploring the mechanism and kinetics of nucleation processes: from crystallization to cavitation	**I-113**	*Roland Mitric* Light-induced nonadiabatic dynamics: from isolated molecules to molecular assemblies and light-harvesting nanostructures	**I-123**	*Ilaria Ciofini* New tools for the description of excited states of molecular systems in complex environment
15:00	**I-074**	*Yitzhak Apeloig* Isomerization mechanisms around E=E′ (E,E′=C,Si) bonds. Experiment and theory	**I-084**	Jeppe Olsen Wave functions with several sets of optimized orbitals	**I-094**	Dage Sundholm Numerical electronic structure theory methods for massively parallel computations on molecules	**I-104**	*Christine Peter* A multiscale simulation perspective on mineralization processes	**I-114**	*Ivano Tavernelli* New strategies for non-adiabatic dynamics with trajectories	**I-124**	*Satoshi Maeda* Artificial force induced reaction (AFIR) method for automated search of adiabatic and nonadiabatic pathways
15:25	**I-075**	*Kendall Houk* Dynamics of pericyclic reactions	**I-085**	John Stanton Active thermochemical tables: what they are, why I care about them, and why you should	**I-095**	*Petr Čársky* Fourier transform of 1/r on graphical processing units – promising tool for applications in nanolithography	**I-105**	*Alexander Nemukhin* Computational modeling of molecular processes in proteins	**I-115**	*Graham Worth* Quantum dynamics simulations of photo-excited molecules using the MCTDH method	**I-125**	*Henrik Koch* The curious case of conical intersections in coupled cluster theory
15:50 – 16:20	COFFEE BREAK											

Time	Philharmonic Hall		Carl-Orff Hall		Black Box		Small Concert Hall		Carl-Amery Hall		Multipurpose Room	
16:20 – 18:25	Contributed Session 1 *Chair: David Tozer*		Contributed Session 2 *Chair: Sotiris Xantheas*		Contributed Session 3 *Chair: Jörn Manz*		Contributed Session 4 *Chair: William Hase*		Contributed Session 5 *Chair: Kaori Fukuzawa*		Contributed Session 6 *Chair: Henk Eshuis*	
16:20	**C-011**	*Georg Schreckenbach* Modeling of two-dimensional (2D) materials: influence of chemical modifications	**C-021**	*Thomas Kühne* The name is bond - hydrogen bond	**C-031**	*Shirin Faraji* Utilizing light for repair of light-induced DNA damages: clever mode of action of DNA photolyases	**C-041**	*Manabu Sugimoto* First-principles molecular dynamics simulations on ammonia synthesis and decomposition	**C-051**	*Andreas Hauser* Carbon nanotubes immersed in superfluid helium: An incomplete flooding due to quantum effects	**C-061**	*Mercedes Alonso* Conductance switching in expanded porphyrins through aromaticity and topology changes
16:35	**C-012**	*Lorenzo Maschio* Local correlation for crystalline solids: dual basis sets by projection in the reciprocal space	**C-022**	*Tristan Bereau* High-throughput screening of drug-membrane thermodynamics	**C-032**	*Oliver Kühn* Ultrafast spin-flip dynamics in transition metal complexes triggered by soft X-ray light	**C-042**	*Tetsuya Taketsugu* Reaction-path bifurcation analyses based on Valley-Ridge transition and global reaction route mapping	**C-052**	*Raul Alvarez-Idaboy* The role of acid-base equilibria in formal hydrogen transfer reactions: uric acid with tryptophanyl radical	**C-062**	*Daniel Aravena* Spin-dependent transport and magnetoresistance in metallo-porphyrin-based supramolecular wires at room temperature
16:50	**C-013**	*Marek Sierka* Density functional theory for periodic systems using density fitting and continuous fast multipole method	**C-023**	*Ragnar Bjornsson* New insights into nitrogenase: QM/MM broken-symmetry DFT studies of FeMoco and the P-cluster	**C-033**	*Debashree Ghosh* Photoprotection mechanism in eumelanin	**C-043**	*Mark Waller* Retrosynthesis and reaction prediction with deep neural networks	**C-053**	*Albeiro Restrepo* Thermodynamics of the partition of Ibuprofen in a lipid bilayer	**C-063**	*Alexandre Magalhães* Catalyzing chemical reactions inside carbon nanotubes
17:05	**C-014**	*Joao B. L. Martins* Adsorption of glycerol and dihydroxyacetone on CaO and MgO surfaces	**C-024**	*Alister Page* Quantum chemical insights into polymer solvation and hofmeister effects in aqueous and non-aqueous environments	**C-034**	*Daniel Roca-Sanjuán* Chemically-induced excited-state chemistry	**C-044**	*Seiji Mori* Graph theory approach in exploration of reaction path networks: Rh(I)BINAP-catalyzed isomerization of allylic amine	**C-054**	*Alessandro Contini* Automatization of the Nwat-MMGBSA method to rescore docking results in medium-throughput virtual screening applications	**C-064**	*Michal Straka* Theoretical calculations of endohedral fullerenes: from chemical bonding to single-molecule switches
17:20	**C-015**	*Wolfgang Hieringer* Electronic structure of molecules at metal surfaces: recent results on organic molecules and coordination compounds	**C-025**	*Olaf Wiest* The past, present, and future of Q2MM	**C-035**	*Bo Durbeej* Exploiting excited-state aromaticity for the design of efficient light-driven rotary molecular motors	**C-045**	*Woo Youn Kim* Automated searching method for reaction paths using molecular graphs and chemical reaction network	**C-055**	*Przemyslaw Dopieralski* Stressed disulfide bonds in alkaline solution	**C-065**	*Matthias Lein* Structural and electronic properties of carbon nano-onions
17:35	**C-016**	*Ralf Tonner* Explaining organic chemistry at surfaces with energy decomposition analysis	**C-026**	*Dmitry Nerukh* Hybrid molecular dynamics - hydrodynamics modelling of liquid solutions: whole virus at atomistic resolution	**C-036**	*László Turi* Electronic excited state lifetimes of anionic water clusters: a quantized time correlation function approach	**C-046**	*Anoop Ayyappan* Exploring chemical evolution using tabu-search based automated reaction finding algorithm	**C-056**	*Joonkyung Jang* Wetting behavior of a surface decorated with periodic pillars	**C-066**	*Juan F. Espinal* Nickel effect on the spacing of 002 plane in a graphite-like structure
17:50	**C-017**	*Antti Karttunen* Crystal structure prediction of inorganic-organic coordination polymers	**C-027**	*Laurence Leherte* Reduced point charge models of proteins - influence of protein-solvent interactions	**C-037**	*Luca De Vico* How to control the absorption wavelength of light harvesting complexes	**C-047**	*Wolfgang Quapp* Patterns of moving saddle points in catalysis and mechanochemistry	**C-057**	*Petra Imhof* Communication in proteins and protein-substrate complexes	**C-067**	*Oscar Lung Wa Chung* Mechanistic insights on Ni-catalyzed selective C-O activation & Cu-catalyzed reductive CO2 coupling to form oxalate
18:05	**C-018**	*Jon M. Matxain* Transition metal doped magnetic Zn12S12 nanoparticles	**C-028**	*Xabier Lopez* Insights into the structural toxicity of aluminum with biomolecules, using a computational approach	**C-038**	*Valérie Brenner* Excited states deactivation in model proteins chains: Nonadiabatic dynamics simulations and ab initio methods	**C-048**	*Michael Springborg* On the theoretical optimization of properties	**C-058**	*Wieslaw Nowak* Camphore's and Huperzine's adventures in proteinland	**C-068**	*Amalia I. Poblador Bahamonde* Mechanistic investigation on the Pd-catalyted hydrogenation of 1,6-enynes: a DFT approach
18:20 – 20:00	DINNER BREAK											
20:00 – 22:00	Poster Session 1 – *supported by ACS Energy Letters*											

Time	Philharmonic Hall	Carl-Orff Hall	Black Box	Small Concert Hall	Carl-Amery Hall	Multipurpose Room
09:00 – 09:40	**PL-6** Plenary Session D *Chair: Josef Michl* *Giulia Galli* Electrochemistry meets condensed matter physics: first principles simulations of photo-catalytic materials					
09:40 – 10:10	COFFEE BREAK					
10:10 – 12:15	Invited Session 13 *Chair: Teresa Head-Gordon*	Invited Session 14 *Chair: Arne Lüchow*	Invited Session 15 *Chair: Regina de Vivie-Riedle*	Invited Session 16 *Chair: Attila Császár*	Invited Session 17 *Chair: Roland Mitric*	Invited Session 18 *Chair: Christine Peter*
10:10	**I-131** *Walter Thiel* Semiempirical quantum chemistry: methodology and excited-state dynamics	**I-141** *Ali Alavi* Recent developments and applications of full configuration interaction quantum Monte Carlo	**I-151** Leticia González Photostability and photodamage in DNA building blocks	**I-161** *Joel Bowman* Many-body potentials for water and protonated water clusters and VSCF/VCI calculations of IR spectra	**I-171** *Fernando Martin* Attochemistry: imaging and controlling electron dynamics in molecules	**I-181** *Zexing Cao* Global simulation of cyanohydrin cleavage by hydroxynitrile lyases
10:35	**I-132** *Stefan Grimme* Applications of the extended tight binding method (GFN-xTB)	**I-142** *Seiichiro Ten-no* Multi-state effective Hamiltonian and size-consistency corrections for stochastic configuration interactions	**I-152** Roland Lindh Non-adabatic chemiluminescent dynamics of the methyl-substituted 1,2-dioxetanes	**I-162** *Robert Berger* What molecules can reveal about fundamental interactions	**I-172** *Shaul Mukamel* Novel multidimensional spectroscopy of conical intersections with X-ray pulses and quantum light	**I-182** *Tim Clark* Metadynamics simulations of G-protein coupled receptors
11:00	**I-133** *Frank Jensen* Developing improved force fields	**I-143** *Roi Baer* Stochastic orbitals for electronic structure and quantum chemistry	**I-153** *Chantal Daniel* Simulation of ultrafast excited state dynamics in transition metal complexes	**I-163** *R. Benny Gerber* Computational vibrational spectroscopy: anharmonic algorithms and determination of 3D structures of biomolecular conformers	**I-173** *H. Bernhard Schlegel* Angular dependence of ionization by short, intense pulses of linear and circularly polarized light	**I-183** *Markus Meuwly* Quantitative atomistic simulations for chemical and biological applications
11:25	**I-134** *Siewert-Jan Marrink* Computational microscopy of (bio) molecular processes	**I-144** *David Tannor* New formulation of quantum mechanics using complex trajectories: application to nonadiabatic transitions and optical excitation	**I-154** *George Schatz* Theories of SERS, TERS, electrochemistry and plasmon-enhanced energy transfer	**I-164** *Lorenz S. Cederbaum* On systems with and without excess energy in environment ICD and other interatomic mechanisms	**I-174** *Peter Saalfrank* Light-driven processes in molecular systems: from photophysics to photochemistry	**I-184** *Sereina Riniker* Replica-exchange enveloping distribution sampling (RE-EDS) to calculate relative binding free energies
11:50	**I-135** *Jan H. Jensen* Using semiempirical methods for fast and automated predictions	**I-145** *Mark Gordon* Dispersion in intermolecular interactions	**I-155** *Joseph Subotnik* Electrochemistry and non-adiabatic dynamics at metal surfaces: the importance of electron-electron correlation	**I-165** *Sergey Yurchenko* Theoretical molecular line lists for atmospheric characterizations of exoplanets	**I-175** *Peter Knowles* On the perturbative computation of ionization energies	**I-185** *Xuhui Huang* Kinetics-controlled molecular self-assembly processes elucidated by kinetic network models
12:15 – 13:45	LUNCH BREAK					

Time	Philharmonic Hall		Carl-Orff Hall		Black Box		Small Concert Hall		Carl-Amery Hall		Multipurpose Room	
13:45 – 15:50	Invited Session 19 *Chair: Johan Åqvist*		Invited Session 20 *Chair: Trygve Helgaker*		Industry Session 1 - *supported by BASF* *Chair: Ansgar Schäfer*		Invited Session 21 *Chair: Markus Meuwly*		Invited Session 22 *Chair: Odile Eisenstein*		Invited Session 23 *Chair: Gregory Beran*	
13:45	**I-191**	*Teresa Head-Gordon* New methods and models for condensed phase simulation	**I-201**	*Don Truhlar* Recent progress in density functional theories	**IN-1**	*Peter Deglmann* The challenge of chemical thermodynamics and kinetics for real world	**I-211**	*Michele Parrinello* Enhanced sampling for chemistry	**I-221**	*Elfi Kraka* A comprehensive view on the Claisen rearrangement of chorismate via a new quantum chemical toolbox	**I-231**	*Takeshi Yanai* Projector augmented wave method incorporated into Gauss-type atomic orbital based density functional theory
14:10	**I-192**	*Jiali Gao* Methods and applications of multistate density functional theory (MSDFT)	**I-202**	*Carlo Adamo* Non-empirical double-hybrid functionals: more theoretical constrains, better performances?	**IN-2**	*Christoph Taeschler* Mechanistic aspects of high temperature reactions of acetonitrile	**I-212**	*Ulf Ryde* Comparison of quantum-mechanical approaches to calculate ligand-binding affinities with free-energy perturbation	**I-222**	*Gabriel Merino* Massive search of planar hyper-coordinate carbon atoms	**I-232**	*Claudia Draxl* From evaluation of methodology to error bars in computational materials science
14:35	**I-193**	*Modesto Orozco* DNA. A fascinating multiscale problem	**I-203**	*Kieron Burke* Reliable DFT results for spin-crossover complexes	**IN-3**	*Michael Edmund Beck* Digging deep into binding modes in protein-Ligand-complexes by quantum chemistry	**I-213**	*Zhipan Liu* Automated reaction pathway sampling using stochastic surface walking method for predicting chemical reactions	**I-223**	*Raghavan B. Sunoj* Non-covalent interactions in asymmetric catalysis: a mechanistic voyage from rationalizations to predictions	**I-233**	*Beate Paulus* The method of increments applied to weakly bound systems
15:00	**I-194**	*Shina Caroline Lynn Kamerlin* Dynamics, flexibility, cooperativity and the evolution of enzyme function	**I-204**	*G Narahari Sastry* Cooperativity of non-covalent interactions	**IN-4**	*Marcel Verdonk* The use of scoring functions for structure-based drug discovery	**I-214**	*GuanHua Chen* Time-dependent density-functional theory for open system and its applications	**I-224**	*Gopalan Rajaraman* Are single molecule magnets predictable? Learning from Ab-initio calculations on lanthanide and transition metal molecular-magnets	**I-234**	*Krzysztof Szalewicz* Physics-based intermolecular potentials for material design
15:25	**I-195**	*Helmut Grubmüller* Towards a mechanistic understanding of ribosomal function	**I-205**	*David Sherrill* Large datasets for benchmarking noncovalent interactions	**IN-5**	*Thomas Fox* Free energy calculations in drug design	**I-215**	Michele Pavanello Real and imaginary-time electron dynamics of open quantum subsystems	**I-225**	*Laura Gagliardi* Computationally guided discovery of metal-decorated metal-organic frameworks active for catalysis	**I-235**	*WanZhen Liang* Analytic energy gradient and hessian of TD-DFT/MM excited-state: implementation and applications
15:50 – 16:20	COFFEE BREAK											

Time	Philharmonic Hall	Carl-Orff Hall	Black Box	Small Concert Hall	Carl-Amery Hall	Multipurpose Room
16:20 – 18:20	Contributed Session 7 *Chair: Kieron Burke*	Contributed Session 8 *Chair: Max Holthausen*	Industry Session 2 - *supported by BASF* *Chair: Robert Franke*	Contributed Session 9 *Chair: Daniel Escudero*	Contributed Session 10 *Chair: Woo Youn Kim*	Contributed Session 11 *Chair: Iris Antes*
16:20	**C-071** *Mario Piris* NOF-MP2: a global method for the electron correlation	**C-081** *Andrey Rogachev* Trianionic corannulene: tunning stability of supramolecular aggregates with alkali metal size	**IN-6** *Glenn Jones* Industrial applications of first-principles modelling to obtain quality measures for screening of catalyst materials	**C-091** *Masayoshi Nakano* Quantum master equation approach to singlet fission dynamics in molecular aggregates	**C-101** *Mercè Deumal* Unraveling the magnetic transition temperature from changes in spin correlation	**C-111** *Ferran Feixas* Accelerating metal-directed protein folding and molecular recognition with enhanced sampling techniques
16:35	**C-072** *Heather Kulik* Recovering the flat plane condition in electronic structure theory at semi-local density functional theory cost	**C-082** *Carsten Baldauf* About underappreciated, yet active conformations of thiourea organocatalysts		**C-092** *Carmen Herrmann* Pathways in molecular conductance and spin coupling	**C-102** *Nathalie Guihery* The magnetic couplings sensitivity to Fock exchange in DFT is not due to spin over-delocalization	**C-112** *Snezana Zaric* Role of aromatic, aliphatic and backbone interactions in the stability of amyloids
16:50	**C-073** *Pierre-François Loos* Dressing the CI matrix with explicit correlation	**C-083** *Brian Yates* A new mechanism for gold catalysis	**IN-7** *Hanne Falsig* A complete reaction mechanism for standard and fast SCR of NOx on VOx/TiO2(001) catalysts	**C-093** *Takatoshi Fujita* Exciton dynamics in organic optoelectronic materials	**C-103** *Annika Bande* Quantum dot inter-Coulombic decay governed by the quantum size effect	**C-113** *Vladimir Palyulin* Design of AMPA receptor positive allosteric modulators: QSAR studies, virtual screening, and molecular dynamics simulations
17:05	**C-074** *Henk Eshuis* Performance of the random phase approximation for first-row transition metal catalysis	**C-084** *Hélène Bolvin* Magnetic coupling between F magnetic centers		**C-094** *Paula Homem-de-Mello* Photophysical properties of macrocycles: a computational and experimental study	**C-104** *Martin Rahm* Ternary gold hydrides: a new class of stable and potentially superconducting compounds	**C-114** *José Pedro Cerón-Carrasco* AQUILES web server: open the eyes to blind docking
17:20	**C-075** *Jiri Klimes* Highly accurate binding energies from the random phase approximation with singles corrections	**C-085** *Masato Kobayashi* Study on metal nanocluster catalysts based on quantum chemical calculation and informatics	**IN-8** *Martin Letz* Investigations on SiO2 glasses to answer the question:"What is a ´good´ glass structure?"	**C-095** *Tangui Le Bahers* Modeling the photochromism of sulphur-doped sodalites using DFT, TD-DFT and SAC-CI methods	**C-105** *Ian Mackinnon* Density functional theory as a predictive tool for superconductivity	**C-115** *Niels Hansen* Thermodynamics of self-assembly of perylene derivatives
17:35	**C-076** *Eduard Matito* Separation of dynamic and nondynamic correlation	**C-086** *Lubomír Rulíšek* Calibrating aurophilic interactions in weakly bound [L-Au-X]…[L'-Au-X] dimers by experiment and theory	**IN-9** *Matthias Bremer* Increasing the polarity of liquid crystals - synthesis and computations	**C-096** *Basile F. E. Curchod* Shedding light on the approximations underlying Ab initio multiple spawning	**C-106** *Fernando Ruipérez* Design of new disulfide-based organic compounds for the improvement of self-healing materials	**C-116** *Janos Daru* Solvation in 2D: microsolvated ions on inert surfaces
17:50	**C-077** *Jan Řezáč* Describing non-covalent interactions in semiempirical QM methods: state of the art and future	**C-087** *Zahra Jamshidi* Surface-enhanced Raman spectroscopy due to charge-transfer chemical mechanism: effect of surface and electric field		**C-097** *William Glover* Polarizable QM/MM for excited-state dynamics	**C-107** *Toyokazu Ishida* Computational modeling of thermal energy storage materials	**C-117** *Allan East* Aqueous solution thermodynamics: a demonstration of effective use of the semicontinuum (cluster + continuum) idea
18:05	**C-078** *Ekaterina Pas* A new spin ratio scaled MP2 (SRS-MP2) method for the prediction of intermolecular interactions	**C-088** *Jean Christophe Tremblay* Irreversible tautomerization in porphycene on Cu(111) induced by scanning tunnelling microscopy	**IN-10** *Thomas Eckl* Automated high-throughput DFT simulations for the development of enhanced energy storage and energy conversion materials	**C-098** *Matthias Stein* Hydrogen conversion in [NiFe]-enzymes and bio-inspired complexes	**C-108** *Eliseo Ruiz* Spin crossover complexes: a challenge from theory to single-molecule devices	**C-118** *Ole Swang* Towards reliable computed thermodynamic data for aqueous metal ions: the case of cadmium
18:20 – 20:00	DINNER BREAK					
20:00 – 22:00	Poster Session 2– *supported by The Journal of Physical Chemistry*					

Time	Philharmonic Hall	Carl-Orff Hall	Black Box	Small Concert Hall	Carl-Amery Hall	Multipurpose Room
09:00 – 09:40	PL-7 Plenary Session E *Chair: Peter Richard Schreiner* Pavel Hobza Noncovalent interactions: theory and applications					
09:40 – 10:10	COFFEE BREAK					
10:10 – 12:15	Invited Session 24 *Chair: Mark Gordon*	Invited Session 25 *Chair: Gernot Frenking*	Invited Session 26 *Chair: Guan Hua Chen*	Invited Session 27 *Chair: Martin Kaupp*	Invited Session 28 *Chair: Qiang Cui*	Invited Session 29 *Chair: Dominika Zgid*
10:10	I-241 *Alán Aspuru-Guzik* Quantum computation for quantum chemistry	I-251 Sason Shaik Oriented electric fields as future smart reagents in chemistry	I-261 Karsten Reuter Refining first-principles photo-electrocatalysis	I-271 *David Tozer* Exchange-correlation functionals from density scaling	I-281 *Marcus Elstner* Multi-scale methods for electron and exciton transfer in biological and organic materials	I-291 *Bogumil Jeziorski* Theoretical determination of properties of helium for new temperature and pressure standards
10:35	I-242 *Michele Ceriotti* Machine-learning unifies the modelling of materials and molecules	I-252 Clémence Corminboeuf Bringing volcano plots as a tool to understand and predict homogenous catalysts	I-262 Fabrizia Negri Challenges in modeling electronic structure, optical and transport properties of conjugated molecular materials	I-272 *Hannes Jonsson* Self-interaction corrected energy functional applied to molecules and solids	I-282 *Elena Laura Coitiño Izaguirre* Sulfenic acid or sulfenate? A matter of protein environment and water access in oxidized Cysteine sites of physiological relevance	I-292 *Manuel Yáñez* Spontaneous generation of radicals and design of anion sponges through Beryllium bonds
11:00	I-243 *Markus Reiher* Interactive and automated exploration of reaction mechanisms	I-253 Julia Rice Nucleobases: from the prebiotic world to self-healing polymers	I-263 *Mariachiara Pastore* From dye-sensitized TiO2 to dye-Sensitized NiO heterointerfaces: a new challenge for theory	I-273 *Julien Toulouse* Combining density-functional theory and many-body methods	I-283 *Matthias Heyden* Solvation and solvent-mediated driving forces: Spatially resolved information from detailed atomistic trajectories	I-293 *Johannes Kästner* Improvements of instanton theory to simulate atom tunneling in astrochemical reactions
11:25	I-244 *Matthias Scheffler* Big data of the chemical physics of materials: discovering interpretable patterns, correlations and causality	I-254 *Matthias Bickelhaupt* Rational design of chemical reactions	I-264 *Biswarup Pathak* Atomistic modeling of nanocluster based electrodes for fuel cell applications	I-274 *Erin R. Johnson* Dispersion interactions from the exchange-hole dipole moment	I-284 *Ville Kaila* Deciphering molecular mechanisms of energy-converting proteins from simulations across scales	I-294 *Eluvathingal D. Jemmis* Borophenes, borospherenes, boranes, 3D-boron allotropes and boron-rich solids
11:50	I-245 *Gregory Voth* Ultra-coarse-graining and its applications	I-255 William Hase Development and applications of direct Dynamics simulations	I-265 *Zhigang Shuai* Understanding intramolecular singlet fission process in D-A polymer from correlated wave-function perspective	I-275 *Matthias Ernzerhof* Factorizations of the exchange-correlation hole	I-285 *Holger Gohlke* Efficient approximation of configurational entropy changes upon binding to biomolecules	I-295 *Péter G. Szalay* On the accuracy of coupled-cluster-type methods describing excited states
12:15 – 13:00	LUNCH BREAK					
13:00 – 20:00	**EXCURSIONS**					
20:00 – 22:00	**Löwenbräukeller** (Address: Nymphenburger Str. 2) **CONGRESS DINNER**					

Time	Philharmonic Hall	Carl-Orff Hall	Black Box	Small Concert Hall	Carl-Amery Hall	Multipurpose Room
09:00 – 09:40	PL-8 Plenary Session F *Chair: So Hirata* *Hiroshi Nakatsuji* Exact general theory for solving Schrödinger equations of atoms and molecules: Free-complement theory and applications					
09:40 – 10:10	COFFEE BREAK					
10:10 – 12:15	Invited Session 30 *Chair: Asbjörn Burow*	Invited Session 31 *Chair: Manuel Yáñez*	Invited Session 32 *Chair: Luca Frediani*	Invited Session 33 *Chair: Christof Hättig*	Invited Session 34 *Chair: Bogumil Jeziorski*	Invited Session 35 *Chair: Zexing Cao*
10:10	**I-301** *Filipp Furche* Recent developments in random phase approximation methods	**I-311** *Josef Michl* Oligosilanes: intuitive understanding of σ delocalization in loose and localization in tight helical conformations	**I-321** *Chiara Cappelli* A fully polarizable embedding model for molecular spectroscopy of aqueous solutions	**I-331** *Anna Krylov* Visualizing the contributions of virtual states to two-photon absorption cross-sections	**I-341** *Rodney J. Bartlett* Quantitative molecular orbital theory	**I-351** *Pedro Fernandes* Nanosecond-timescale conformational dynamics of enzymes, and its impact on reaction rates
10:35	**I-302** *Axel Becke* Vertical excitation energies from the adiabatic connection	**I-312** *Gernot Frenking* Aspects of chemical bonding	**I-322** *Jacob Kongsted* Excited states in complex systems through polarizable (density) embedding	**I-332** *Xiaosong Li* Two-component non-collinear time-dependent spin density functional theory for electronic dynamics and excited state calculations	**I-342** *Andreas Köhn* Applications of interenally contracted multireference coupled-cluster theory	**I-352** *Yiqin Gao* Computer simulations of chemical reactions in solution
11:00	**I-303** *Eunji Sim* Reliable DFT results with density correction	**I-313** *Marco Nascimento* Are one-electron bonds any different from standard two-electrons covalent bonds?	**I-323** *Lyudmila Slipchenko* Polarizable embedding and beyond: modeling photoactive proteins with the effective fragment potential method	**I-333** *Andreas Dreuw* Algebraic diagrammatic construction - a versatile approach to excited states, ionization potentials and electron affinities	**I-343** *Shuhua Li* Advances in Electronic Structure Methods for Strongly Correlated Systems and Condensed Phase Systems	**I-353** *Young Min Rhee* Simulating photo-excited dynamics of biological complexes: overcoming present challenges with interpolated potentials
11:25	**I-304** *Andreas Görling* Density-functional methods with the accuracy and wide applicability of high-level multi-reference approaches	**I-314** *Julia Contreras-García* A new model for reference densities - really getting rid of interactions	**I-324** *Fred Manby* Multiscale embedding methods for accurate quantum chemistry of complex systems	**I-334** *Spiridoula Matsika* Theoretical studies of the interaction of uracil with low energy electrons	**I-344** *Jiri Pittner* DMRG-externally-corrected local pair natural orbital based coupled cluster method	**I-354** *Carmay Lim* How native and alien metal cations bind ATP
11:50	**I-305** *Paul Ayers* Variational principle for partitioning molecules into atomic contributions	**I-315** *Russell J. Boyd* Insight into hydrogen-bonded clusters and noncovalent interactions from changes in atomic energies	**I-325** *Kurt V. Mikkelsen* Exploitation of solar energy	**I-335** *John Herbert* First-principles exciton models, with application to singlet fission	**I-345** *Ove Christiansen* Tensor decomposition and coupled cluster theory	**I-355** *David Smith* A multiscale computational investigation of SILPcatalysis: the water-gas shift reaction
12:15 – 13:45	LUNCH BREAK					

Time	Philharmonic Hall		Carl-Orff Hall		Black Box		Small Concert Hall		Carl-Amery Hall		Multipurpose Room	
13:45 – 15:50	Invited Session 36 *Chair: Jiali Gao*		Invited Session 37 *Chair: Filipp Furche*		Invited Session 38 *Chair: Julien Toulouse*		Invited Session 39 *Chair: Francesco Aquilante*		Invited Session 40 *Chair: Andreas Dreuw*		Invited Session 41 *Chair: Brian Yates*	
13:45	**I-361**	*Richard Henchman* Theory for the entropy of liquid mixtures of flexible molecules	**I-371**	*Marcel Nooijen* Towards a local coupled cluster theory for solids	**I-381**	*So Hirata* Many-body Green´s function theory: algebraic recursions, linked- and irreducible-diagram theorems, and general-order algorithms	**I-391**	*Toru Shiozaki* On-the-fly CASPT2 surface hopping dynamics	**I-401**	*Patrick Norman* Response theory techniques to address X-ray spectroscopies	**I-411**	*Igor Alabugin* Reinventing cycloaromatization reactions: the diradical /zwitterion dichotomy
14:10	**I-362**	*Johan Åqvist* Entropy and enzyme catalysis	**I-372**	*Georg Kresse* The relation between the random phase approximation and GW and analytic forces for the RPA	**I-382**	*Dominika Zgid* Green´s function embedding methods	**I-392**	*David Tew* Quantum dynamics on accurate electronic potentials	**I-402**	*Daniel Crawford* Streamlining coupled cluster response theory	**I-412**	*Miroslav Urban* DFT study of the Au-C bond formation in gold implanted polyethylene
14:35	**I-363**	*Qiang Cui* Understanding metalloenzyme catalysis with QM/MM free energy simulations	**I-373**	*Silke Biermann* Electronic structure calculations for correlated electron materials: a dynamical mean field perspective	**I-383**	*Denis Jacquemin* Is BSE/GW an effective method for modeling optical spectra of molecules?	**I-393**	*Yuki Kurashige* Ab initio modeling of inter-molecular electronic transition processes in molecular aggregates	**I-403**	*Benoît Champagne* Towards investigating the optical properties of molecular and ionic crystals using multi-scale approaches	**I-413**	*Attila Császár* Astructural molecules
15:00	**I-364**	*Pavel Jungwirth* Cell penetration and membrane fusion: two sides of the same coin	**I-374**	*Volker Blum* Affordable high numerical accuracy for large molecules and materials from numeric atom-centered basis functions	**I-384**	*Lucia Reining* Quasi-particles and satellites from a direct approach to the calculation of many-body Green´s functions	**I-394**	*Hans Jørgen Aagaard Jensen* Open-shell MC-srDFT - a new way to describe high-spin, low-spin, intermediate spin states and more	**I-404**	*Sonia Coriani* Developing theoretical "beam-lines" for modern experiments	**I-414**	*Annia Galano* The role of acid-base equilibria in the antioxidant and pro-oxidant activity of phenolic compounds
15:25	**I-365**	*Gerhard Hummer* Molecular simulations of lipid membrane sensing and remodeling dynamics	**I-375**	*Gregory Beran* Ab initio molecular crystallography: Aiding and abetting experiment	**I-385**	*Wim Klopper* Using the GW and Bethe-Salpeter methods in molecular quantum chemistry	**I-395**	*Piotr Piecuch* Stochastic CC(P;Q) theory: converging high-level coupled-cluster energetics by Monte Carlo sampling and moment expansions	**I-405**	*Antonio Rizzo* Electronic nonlinear spectroscopies: recent contributions of theory and computational science	**I-415**	*Munir Skaf* Thermodynamic forces between plant cell wall constituents
15:50 – 16:20	COFFEE BREAK											

Time	Philharmonic Hall		Carl-Orff Hall		Black Box		Small Concert Hall		Carl-Amery Hall		Multipurpose Room	
16:20 – 18:20	Contributed Session 12 *Chair: David Tew*		Contributed Session 13 *Chair: Wolfgang Domcke*		Contributed Session 14 *Chair: Andy Teale*		Contributed Session 15 *Chair: Reinhold Fink*		Contributed Session 16 *Chair: Tanya K. Todorova*		Contributed Session 17 *Chair: Marco Nascimento*	
16:20	**C-121**	*Jan M.L. Martin* Explicitly correlated benchmark study on water clusters: The right answer for the right reason?	**C-131**	*Nick Mayhall* Multiexcitons and strong correlation via single-excitation wavefunctions: applications and future directions	**C-141**	*Stella Stopkowicz* Accurate treatment for ground and excited states of atoms and molecules in strong magnetic fields	**C-151**	*Martin Kaupp* Mixed valency and local hybrid functionals	**C-161**	*Mark Iron* Computational insights into sulphur isotopic fractionation in carbonate-associated sulphate	**C-171**	*José Enrique Barquera-Lozada* Aromaticity from the point of view of the vorticity of the current density tensor
16:35	**C-122**	*Ricardo Mata* GöBench: a joint initiative for experimental benchmarking of quantum chemical methods	**C-132**	*Remco Havenith* The computation of dielectric constants	**C-142**	*Sandra Luber* Recent advances in theoretical spectroscopy from ab initio molecular dynamics	**C-152**	*Lars Goerigk* Double-hybrid density functionals: is there anything new to tell?	**C-162**	*Sílvia Simon* Tailoring resonance assisted hydrogen bonds	**C-172**	*Fabio Pichierri* Cesium cation-π interactions: DFT and QTAIM studies
16:50	**C-123**	*Peter Nagy* Approaching CCSD(T)/CBS energies for large molecules with the linear-scaling local natural orbital CCSD(T) method	**C-133**	*Andrzej L. Sobolewski* Organic photovoltaics with p-f-n junctions: computational study of ferroelectric columnar molecular clusters	**C-143**	*Malgorzata Biczysko* Anharmonic effects on vibrational spectra intensities: infrared, Raman, vibrational circular dichroism, and Raman optical activity	**C-153**	*Sergei Vyboishchikov* Exchange-Correlation Potentials and Energy Densities in Spherically Confined Atoms	**C-163**	*Ulrike Salzner* Effect of biradical character of organic molecules on Opto electronic properties	**C-173**	*András Stirling* Hypervalency and reactivity from Wannier orbitals
17:05	**C-124**	*Graham Fletcher* Large-scale valence bond applications: excitons and transition metal complexes	**C-134**	*Thomas Koerzdoerfer* Accurate ionization potentials, electron anities, and photoelectron spectra of molecules from first principles	**C-144**	*Takeshi Iwasa* Infrared absorption spectroscopy beyond the dipole approximation based on the multipolar Hamiltonian: Theory and application	**C-154**	*Arindam Chakraborty* Linked-cluster formulation of screened electron-hole interaction from explicitly-correlated geminal functions without using unoccupied states	**C-164**	*Hong-Xing Zhang* Computationally driven design of efficient photosensitizer for dye-sensitized solar cell applications	**C-174**	*Leonardo Belpassi* Charge-displacement analysis: a simple tool to reveal charge transfer effects throughout the whole periodic table
17:20	**C-125**	*Jean-Philip Piquemal* Scalable polarizable molecular dynamics using Tinker-HP: millions of atoms on thousands of cores	**C-135**	*Emanuele Coccia* Dissipation and dephasing for molecules close to plasmonic nanoparticles: an ab initio approach	**C-145**	*Franco Egidi* Toward the accurate simulation of vibrationally-resolved spectra for spin-forbidden transitions	**C-155**	*István Mayer* Local spins	**C-165**	*Martial Boggio-Pasqua* Computational studies of the photoswitching mechanisms in photochromic ruthenium complexes	**C-175**	*Apostolos Kalemos* The nature of the chemical bond in Be containing molecules: Be2+,0,-, Be3, Be00,-, BeOBe +,0,-
17:35	**C-126**	*Joonsuk Huh* Vibronic boson sampling	**C-136**	*Robert Góra* Microhydration induces qualitative changes in the photochemistry of biomolecular building blocks	**C-146**	*Sergei Ivanov* Nuclear correlation effects in X-ray spectroscopy from a time-domain perspective	**C-156**	*Fan Wang* Spin-orbit coupling effects of open-shell systems with coupled-cluster theory	**C-166**	*Aurélie Perrier* Photosensitizing properties of functionalized thiolate-protected gold nanoclusters: insights from theory	**C-176**	*David Wilson* Theoretical investigation of a strong cis-effect in an imidazole-imidazolium substituted alkene
17:50	**C-127**	*Luca Frediani* PCMSolver: a modern, modular approach to include solvation in any quantum chemistry code	**C-137**	*Isabelle Navizet* Role of the environment in bioluminescence emission: QM/MM study	**C-147**	*Stepan Sklenak* DFT calculations of NMR parameters of framework and extra-framework atoms in silicon-rich zeolites	**C-157**	*Mikael P. Johansson* Can spin-state energetics of transition metal complexes be accurate at single reference level?	**C-167**	*David Henry* Modifying the reactivity of gallium nanoclusters with ligands	**C-177**	*Ignacy Cukrowski* Fragment attributed molecular system energy change (FAMSEC) in the study of interactions and molecular stability
18:05	**C-128**	*Sebastian Höfener* Combining frozen-density embedding with the conductor-like screening model using Lagrangian techniques	**C-138**	*Stefan Knippenberg* Investigation of optical probes for membrane phase recognition	**C-148**	*Alfonso Hernández-Laguna* Elastic behavior of White Micas solid solutions as a function of the pressure	**C-158**	*Ran Friedman* Specific ion interactions with biomolecules: molecular dynamics simulations and energy decomposition analysis	**C-168**	*Thibaud Étienne* Orbital relaxation and electronic transitions - what is the nature of Handy´s Z-vector?	**C-178**	*Hugo Gattuso* Efficiently modeling the electronic circular dichroism of amino and nucleic acids ensembles
18:20 – 20:00	DINNER BREAK											
20:00 – 22:00	Poster Session 3 – *supported by ACS Publications*											

Time	Philharmonic Hall	
09:00 – 10:20	Plenary Session G *Chair: David Sherrill*	
09:00 – 09:40	**PL-9**	*Francesco Evangelista* Multireference coupled cluster theory, infinities and renormalization
09:40 – 10:20	**PL-10**	*Johannes Neugebauer* Subsystem density-functional theory for properties and spectra of complex chemical systems
10:20 – 10:50	COFFEE BREAK	
10:50 – 12:10	Plenary Session H *Chair: Walter Thiel*	
10:50 – 11:30	**PL-11**	*Ursula Roethlisberger* Next generation first-principles based multiscale simulations: computational chemistry meets artificial intelligence
11:30 – 12:10	**PL-12**	*Frank Neese* Wavefunction based correlation methods for large molecules: recent developments, applications and limitations
12:10 – 12:50	**CLOSING CEREMONY AND POSTER AWARDS**	

POSTER SESSIONS

Poster Session 1 – Monday, 28 August 2017

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PO1-1 Systematic evaluation of optimization strategies used to investigate organic reaction mechanisms in solvent
Gavin Jones, United States

PO1-2 Developing a DFT/TD-DFT method for designing BODIPY based anion sensors and for their mechanism demonstration
Haamid Bhat, India

PO1-3 Orbital phase theory in diastereoselectivity of electrophilic addition to 4-fluoro-1-methyleneadamantane
Yuji Naruse, Japan

PO1-4 Radiative association of 36Ar and 38Ar with ionic hydrogen
Fatima Talhi, Algeria

PO1-5 Thermal activation of methane by a concerted double C-H bond insertion: charge-induced catalysis
Jilai Li, Germany

PO1-6 Optimizing water oxidation with hematite by simulations
Xueqing Zhang, Netherlands

PO1-7 Study of surface reactivity of high index platinum surfaces
Gabriele Tomaschun, Germany

PO1-8 Hybrid algorithm based on tabu search method for the synthesis of macromolecular compounds with imposed properties
Teodora Rusu, Romania

PO1-9 Catalytic roles of metal-bound hydroxide and arginine in pyruvate class-II aldolase investigated by QM/MM metadynamics
Jen-Shiang K. Yu, Taiwan, Republic of China

PO1-10 On the origin of reactivity enhancement/suppression upon sequential ligation: the [Re(CO)x]+/CH4 (x=0X3) couples
Shaodong Zhou, Germany

PO1-11 Theoretical study of Co(II/III)-complex catholytes used Li-ion redox flow batteries
Ji Young Park, Republic of South Korea

PO1-12 Stochastic basis set approach to density functional theory
Marcel David Fabian, Israel

PO1-13 Thermal properties of organic solids from the quasi-harmonic approximation
Gerit Brandenburg, United Kingdom

PO1-14 Ethylene glycole decomposition on a Palladium subnanometric cluster: a graph theory based approach
Remedios Cortese, Italy

PO1-15 A comparative study of hydrogen bond and iminium mechanisms in organocatalytic and enzymatic reduction
David Ferenc, Hungary

PO1-16 Improved accuracy of hybrid atomistic/coarse-grained simulations using reparametrised interactions
Annick Renevey, Switzerland

PO1-17 Binding isotope effects as a tool to detecting HIV-1 RT binding sites
Agnieszka Krzemińska, Poland

PO1-18 Simulation of reversibly interlocked SWCNTs
Sebastian Gsänger, Germany

PO1-19 Indirect-to-direct band gap crossover in few-layer transition metal dichalcogenides
Yajing Sun, China

PO1-20 Interacting quantum atoms approach applied to the S66 database of noncovalent complexes
Dimas Suarez, Spain

PO1-21 Probing feasibility limits of coupled-cluster theory: highly accurate barriers of unexpected reactions for energetic materials
Vitaly Kiselev, Russian Federation

PO1-22 On the nature and reactivity of the substrate/dioxygen intermediate in tyrosinase. QM/MM correlation with spectroscopy
Prokopis Andrikopoulos, Czech Republic

PO1-23 Explicitly correlated N-electron valence state perturbation theory (NEVPT2-F12)
Yang Guo, Germany

PO1-24 Elucidation of the singlet fission mechanism: a theoretical insight
Meilani Wibowo, Netherlands

PO1-25 Polynuclear Li12F13- superhalogen anion as a steric shielding agent with respect to selected metal ions
Marcin Czapla, Poland

PO1-26 Analytic hyperpolarizability and polarizability derivative with fractional occupation numbers for large extended systems
Yoshio Nishimoto, Japan

PO1-27 Trends in catalytic activity of Ni-based electrodes for the hydrogen evolution reaction
Hannah Schlott, Germany

PO1-28 Improving the thermodynamics and transferability of coarse-grained models
Thomas Potter, United Kingdom

Poster Session 1 – Monday, 28 August 2017

supported by ACS Energy Letters

PO1-29 Exploring multistep intersystem crossing pathways of cinnamate-based sunscreens by automated reaction path search methods
Kaoru Yamazaki, Japan

PO1-30 Trajectory surface hopping study of the photodissociation dynamics of phenol
Weiwei Xie, Germany

PO1-31 Reactivity and selectivity of polycyclic aromatic hydrocarbons: shape and size dependence
Israel Fernandez, Spain

PO1-32 Conformational changes induced by fluorination: extended molecular dynamics of unguisin peptides
Natalia Diaz, Spain

PO1-33 Development of the quantitative structure-property relationships (QSPR) for predicting char yield of polybenzoxazines
Maryam Sairi, United Kingdom

PO1-34 Embedding metal atoms in icosahedral structures: biicosahedral metallaboranes as three-dimensional analogues of naphtalene
Alexandru Lupan, Romania

PO1-35 Towards rationalizing the trends in the electronic structure of MX2 3d transition metal dihalide monolayers
Cheng-Chau Chiu, Taiwan, Republic of China

PO1-36 Rapid, accurate, precise and reliable relative free energy prediction using ensemble based thermodynamic integration
Agastya P. Bhati, United Kingdom

PO1-37 Molecular modeling, docking, NBO, and vibrational studies of new αaminophosphonates as antitumor agents targeting MCF7
Mohamed Awad, Egypt

PO1-38 The master factors influencing the potency of BACE-1 alzheimer inhibitors: computational & molecular docking studies
Faten Atlam, Egypt

PO1-39 Maximum probability domains: theoretical foundations and computational algorithms
Guillaume Acke, Belgium

PO1-40 DFT studies on catalytic CO_2 fixation by monoethanolamine
Maneeporn Puripat, Thailand

PO1-41 Tunneling of hydrogen transfer reactions on and in interstellar ices
Thanja Lamberts, Germany

PO1-42 Proton collisions on prebiotic candidates: HCN oligomers
Marie-Christine Bacchus, France

PO1-43 Active site protonation and the reactivation of acetylcholine esterase
Thomas Driant, France

PO1-44 Splitting the Coulomb hole into its dynamic and nondynamic parts
Mireia Via Nadal, Spain

PO1-45 Protein oxidation mechanisms via OH radical
Jon Uranga, Spain

PO1-46 QM/MM investigation of structure-spectroscopy correlations in the intermediate Q of soluble methane monooxygenase
Christine Schulz, Germany

PO1-47 Reaction mechanism of hydrogermylation/hydrostannylation of unactivated alkenes with two-coordinate EII hydrides (E = Ge, Sn)
Lili Zhao, Germany

PO1-48 Influence of semiempirical dispersion correction on the DFT description of inorganic layered compounds: alkaline-earth fluorohalides
Daniel Sethio, Switzerland

PO1-49 Investigation of catalytic dehydrocoupling of dimethylamine-borane by titanocene: a DFT and topologic study
Jingwen Zhu, France

PO1-50 Optimal Faujasite structures for post combustion CO_2 capture in swing adsorption processes
Hector Prats Garcia, Spain

PO1-51 Ni-phosphine bond strengthening trough coordination of the strong σ-donors ECp* (E= Al, Ga)
Julius Hornung, Germany

PO1-52 Effects of interphase region on glass transition temperature of grafted carbon nanotubes reinforced epoxy composites
Chaoyi Peng, China

PO1-53 DLPNO-CCSD(T) scaled methods for the accurate treatment of large supramolecular complexes
Joaquín Calbo, Spain

PO1-54 The molecular mechanism of ligand unbinding from the human telomeric G-quadruplex
Sheh-Yi Sheu, Taiwan, Republic of China

PO1-55 Mechanically controlled electron transfer in a single-polypeptide transistor
Dah-Yen Yang, Taiwan, Republic of China

Poster Session 1 – Monday, 28 August 2017

supported by ACS Energy Letters

PO1-56 DFT study of the selectivity of DOPA-decarboxylase
Emily Harrison, United States

PO1-57 DFT study of the selectivity of monoamine oxidase B (MAOB)
Samantha Jelinek, United States

PO1-58 Design of novel inhibitors for the aldehyde dehydrogenases I: Left orientation
Caroline Magee, United States

PO1-59 DFT analysis of the selectivity of phenylalanine hydroxylase
Madison Perchik, United States

PO1-60 Electron transfer in organic and biological materials
Antoine Carof, United Kingdom

PO1-61 Hydrogen atom abstraction from ethanol by atomic hydrogen in aqueous solution
Suraj Kannath, Poland

PO1-62 Getting ion-protein interactions right in molecular dynamics simulations
Elise Duboué-Dijon, Czech Republic

PO1-63 Design and synthesis of novel inhibitors for the tyrosine hydroxylase enzyme
Rebecca Evans, United States

PO1-64 Tricoordinate boron as donor ligand: bonding and reactivity patterns in iron pincer complexes
Lisa Vondung, Germany

PO1-65 Design of novel inhibitors for the aldehyde dehydrogenases II: Right orientation
Emma Selner, United States

PO1-66 How many water molecules does it take to dissociate the hydrogen halides?
Alba Vargas, Mexico

PO1-68 The reactivity of α-O in Fe-zeolites: a mulitreference aproach
Simon Hallaert, Belgium

PO1-69 Ruthenium-xantphos catalyzed olefin hydrogenation - how well does contemporary DFT predict experimentally observed energy spans?
Markus Hölscher, Germany

PO1-70 Theoretical investigation on the role of non-covalent interactions in a regioselective aryl C(sp2)-H borylation reaction
Anju Unnikrishnan, India

PO1-71 DFT study of CH bond activation of Os+, Ir+, and Pt+ reacting with acetylene
Zikri Altun, Turkey

PO1-72 Insights on chiral induction using (s)-BINOL-phosphoric acids in enantioselective reactions through transition state modeling
Avtar Changotra, India

PO1-73 Generation of parent phenylphosphinidene and its oxidation to phenyldioxophosphorane, the elusive phosphorous analogue of nitrobenzene
Artur Mardyukov, Germany

PO1-74 Effects of solvents and temperature on NMR chemical shifts in hydrogen-bonded complexes
Yukihiro Ota, Japan

PO1-75 Mechanistic insights and origin of stereoinduction on NHC catalysed asymmetric reactions using transition state modelling
Monika Pareek, India

PO1-76 Halogen bonding involving aromatic acceptors
Shi Jun Ang, Singapore

PO1-77 Mechanistic insight into the hydrosilylation of alkenes using early main-group metal catalysts
Holger Elsen, Germany

PO1-78 Mechanistic insights into aqueous methanol dehydrogenation
Vivek Sinha, Netherlands

PO1-79 On the mechanism of silver-catalyzed isomerization of cubane and homocubane
Said Jalife-Jacobo, Mexico

PO1-80 Effect of an external electric field on the structure and dynamics of CaO films
Mikhail S. Kuklin, Finland

PO1-81 Coordination chemistry of Zn2+: tetrahedral coordination or penta-coordination? A DFT analysis and review
Henry Chermette, France

PO1-82 Synthetic nitrogen fixation with mononuclear molybdenum complexes: electronic-structural and mechanistic insights from DFT
Benedikt Flöser, Germany

PO1-83 Effects of external electric field and anisotropic long-range reactivity on charge separation probability
Sangyoub Lee, Republic of Korea

Poster Session 1 – Monday, 28 August 2017

supported by ACS Energy Letters

PO1-84 Activation strain analyses for copper-free click reactions of alkyl azides with cyclooctynes and dibenzocyclooctynes
Felipe De Souza Vilhena, Brazil

PO1-85 Computational study of the electrochemical reduction of [(dpp-bian)Re(CO)3Br]0: mechanism and EPR spectroscopy of intermediates
Alexey Dmitriev, Russian Federation

PO1-86 Non-analytical functionals: a new strategy in density functional theory
Kati Finzel, Belgium

PO1-87 Numerical nuclear second derivatives on a grid: a faster and enabling method for Hessian calculations
Tzuhsiung Yang, United States

PO1-88 A study of the global and local aromaticity of Hetero[8]circulenes
Abulikemu Keremu, China

PO1-89 A study of the global and local antiaromaticity of 1, 4-diazapentalene derivatives
Muhetaer Yimieraishan, China

PO1-90 Time-dependent coupled-cluster method for laser-driven multielectron dynamics
Himadri Pathak, Japan

PO1-91 From G4(MP2)-6X to W3X-L: A Range of Efficient and Accurate Thermochemical Composite Protocols
Bun Chan, Japan

PO1-92 Theoretical study of anatase (101) and rutile (110) TiO2 nanotubes
Gustavo Olinto, Brazil

PO1-93 Ab initio construction of phase diagrams for molecular crystals
Ctirad Cervinka, Czech Republic

PO1-94 Quantum chemical exploration of transition metal mediated CO_2 disproportionation and hydrogenation
Lisa Roy, Germany

PO1-96 Molecular dynamics simulation reveals how phosphorylation of tyrosine 26 of PGAM1 upregulate glycolysis
Yan Wang, China

PO1-97 Purely relativistic electric dipole moment interactions of the electron from quasi-relativistic calculations
Konstantin Gaul, Germany

PO1-98 Steeplechase for 2-RDM approximations
Mauricio Antonio Rodríguez Mayorga, Spain

PO1-99 Excited states insight to assess phototoxicity of non-steroidal anti-inflammatory drugs
Neus Aguilera-Porta, Spain

PO1-100 New porphyrin for application in dye-sensitized solar cells
Cassiano Minoru Aono, Brazil

PO1-101 Systematic search for chemical reactions in gas-phase contributing to methanol formation in the interstellar medium
Victoria Gámez, Mexico

PO1-102 Modeling of ions in aqueous environments: from the gas to the condensed phase
Daniel J. Arismendi Arrieta, Spain

PO1-103 A study of the global and local aromaticity of Azaacepentalenes
Abulimiti Abudoukadeer, China

PO1-104 Recent advances in approximate excited state calculations in the ADF modeling suit
Robert Rüger, Netherlands

PO1-105 Combined theoretical and experimental studies on polymer and plasticizer interactions
Avtar Singh, India

PO1-106 CO, NO, and NO2 adsorptions on boron antisite (BN) in boron-rich boron nitride nanotube (BNNT)
Heechol Choi, Republic of Korea

PO1-107 Structural analysis of phthalocyanines dimers using computational methods
Mateus Zanotto, Brazil

PO1-108 Density functional study of [2+1] radical cation cycloaddition
Xinglong Zhang, United Kingdom

PO1-109 Configurational bias Monte Carlo method to sample molecular flexibility: the case of octane and 1,2-dichloroethane
Henrique Cezar, Brazil

PO1-110 DFT calculations on enantioselective Pd-catalyzed diboration of 1,1-disubstituted allenes: dispersion-drive eantioselectivity
Qinghai Zhou, China

PO1-111 Aluminum interaction with serine and O-phosphoserine
Elena Formoso, Spain

PO1-112 Preparing a computational database of surface structures for investigating catalytic reactions

Poster Session 1 – Monday, 28 August 2017

supported by ACS Energy Letters

Hyun Woo Kim, Republic of Korea

PO1-113 Experimental and theoretical investigations of spectroscopic properties of azobenzene derivatives
Jean-Pierre Dognon, France

PO1-114 Computational thermochemistry of carbamic acid and related compounds
Erdi Bleda, Turkey

PO1-115 The effect of the environment on the photodynamics of biological chromophores
Dmitry Morozov, Finland

PO1-116 A QM/MM study of the catalytic mechanism of human β-ketoacyl reductase
Fabiola Medina, Portugal

PO1-117 Sightseeing in the electronic structure: topological analysis of $|\Psi|2$
Michael Andree Heuer, Germany

PO1-118 Mechanistic studies and bonding situation on organometallic chemistry of gold(III) complexes.
Karinne Miqueu, France

PO1-119 Impact of chosen DFT functionals on one- and two-photon absorption properties of fluorescent proteins chromophores
Dawid Grabarek, Poland

PO1-120 Nitrogen doping strategies for modulating the biradicaloid nature of acenes: insights from multireference calculations
Max Pinheiro Jr, Brazil

PO1-121 Computation of atom-atom electrostatic energy in RNA based on multipolar electrostatics
Yongna Yuan Yuan, China

PO1-122 A computational study of the Diels-Alder reaction between 2,3-dibromo-1,3-butadiene and maleic anhydride
Uxia Rivero, Switzerland

PO1-123 Improved partitioning of biomolecules for quantum-chemical embedding calculations based on graph theory
Mario Wolter, Germany

PO1-124 PEGylation of temozolomide (TMZ): a molecular dynamics study
Tatiana F. Vieira, Portugal

PO1-126 Decoherence of electron dynamics upon ionization of polyatomic molecules
Morgane Vacher, Sweden

PO1-127 Investigation of the degradation process of chlorhexidine using Density Functional Theory calculations
Michele Aparecida Salvador, Brazil

PO1-128 Deep eutectic solvents: the effect of the hydrogen bond donor on structure
Ryan Stefanovic, Australia

PO1-129 How does nitrogen change carbon nanotube chirality? Insights from quantum chemistry
Clothilde Eveleens, Australia

PO1-130 Development and application of ReaxFF for describing catalytic Boron nitride nanotube growth
Ben McLean, Australia

PO1-131 The electronic structure of the [C20X20]-, [C20X20]-2, [Si20F20]-, [Si20F20]-2 (X= F, Cl, Br, I) anions
Slawomir Berski, Poland

PO1-132 From functional mechanism to new therapeutic tools: reaction modelling and computational design of PDC inhibitors
Jacopo Sgrignani, Switzerland

PO1-133 Towards the description of non-covalent interactions in AP1roG model
Filip Brzęk, Poland

PO1-134 CO_2 hydrogenation using earth abundant metal catalysts: role of ligand
Kuber Singh Rawat, India

PO1-135 Instantaneous absorption spectra of firefly oxyluciferin using the first principle molecular dynamics simulations
Nobuaki Koga, Japan

PO1-136 Low-lying excited states and diradical nature of conjugated dicarbonyl compounds
Diego López Carballeira, Spain

PO1-137 Energetics and dynamics of a light-driven sodium-pumping rhodopsin
Carl-Mikael Suomivuori, Finland

PO1-138 Mechanistic study on photocatalytic water splitting with carbon nitride materials
Johannes Ehrmaier, Germany

PO1-139 Fluorescent markers for the detection of amyloid-beta in Alzheimer's disease
Francesca Peccati, Spain

PO1-140 DFT study of Cp*CoIII-catalyzed C–H alkenylation/annulation reactions of indoles with alkynes
Ken Sakata, Japan

PO1-141 Ab initio crystal orbital calculation of electronic structure of B-type model-DNA
Hiroyuki Teramae, Japan

Poster Session 1 – Monday, 28 August 2017

supported by ACS Energy Letters

PO1-142 Computational modeling of versatile photosensitizers
Irene Casademont Reig, Spain

PO1-143 Multistructural microiteration technique for geometry optimization and reaction path calculation in large systems
Kimichi Suzuki, Japan

PO1-144 Nuclear motion is classical
Irmgard Frank, Germany

PO1-145 Heavy atom secondary kinetic isotope effect on tunneling
André K. Eckhardt, Germany

PO1-146 Why lead(II) hydride complex would be better for CO_2 activation than its 14 group analogs?
Nery Villegas-Escobar, Chile

PO1-147 Ab initio molecular dynamics simulations of the ion irradiation on CH4ice
Lenin Díaz, Brazil

PO1-148 Second-order perturbation theory based on density matrix renormalization group: applications for transition metal complexes
Quan Phung, Belgium

PO1-149 XMCQDPT2 calculations elucidated the origin of red to far-red spectral tuning in light-sensitive proteins phytochromes
Egle Maximowitsch, Germany

PO1-150 How do oxidised phospholipids affect the properties of a lipid bilayer?
Alexandra Schumann-Gillett, Australia

PO1-151 Computational study of hydrogen shift reaction catalysed by sulphuric acid in Criegee intermediate
Farzaneh Sarrami Foroushani, Australia

PO1-152 On-the-fly kinetic Monte Carlo based on global reaction route mapping
Izaac Mitchell, Australia

PO1-153 Serenity: a subsystem quantum chemistry program
Jan Unsleber, Germany

PO1-154 Towards laser pulse control of molecular symmetry breaking and restoration
Chunmei Liu, Germany

PO1-155 Combining AIMD and neutron scattering data based EPSR simulations to uncover water participation in catalysis
Nicole Holzmann, United Kingdom

PO1-156 MD simulation analysis on asynchronous solute-solvent coupling magnitude in ring closing reaction of chromene
Yasuhiro Shigemitsu, Japan

PO1-157 Theoretical description of excitations and excitonic couplings of perfluoropentacene
Anna-Katharina Hansmann, Germany

PO1-158 Lowest electronic states of alkali (Li, Na, K, Rb) -- alkaline-earth (Ca, Sr) diatomic molecules
Johann V. Pototschnig, Austria

PO1-159 Global search for periodic structures of carbon by artificial force induced reaction method
Makito Takagi, Japan

PO1-160 Decoherence correction and trivial crossing detection in fragment-orbital based surface hopping
Samuele Giannini, United Kingdom

PO1-161 Adsorption and dissociation of water on tungsten trioxide (001) from first principles
Thomas Teusch, Germany

PO1-162 Water adsorption on tantalum(V) nitride (100): favourite adsorption sites and surface behaviour
Thorben Petersen, Germany

PO1-163 Towards efficient coupled-cluster theories for periodic systems
Theodoros Tsatsoulis, Germany

PO1-164 Intramolecular electronic flux during adiabatic attosecond charge migration
Jörn Manz, Germany

PO1-165 In-silico homovalent screening of hybrid halide perovskite materials for tandem solar cells
Manaswita Kar, Germany

PO1-166 A quasi-diabatization scheme on the study of vibronic coupling of chlorophylls excited states
Petra Shih, Taiwan, Republic of China

PO1-167 Evaluation of the cohesive energy of a solid via lattice sums
Elke Pahl, New Zealand

PO1-168 Molecular dynamics simulation studies of structure and dynamics of poly(acrylic) acid in semidilute concentration regime
Abhishek Kumar Gupta, India

PO1-169 Quantum chemical investigation of the incorporation of Uranium(V) into Magnetite
Robert Polly, Germany

Poster Session 1 – Monday, 28 August 2017

supported by ACS Energy Letters

PO1-170 Quantum chemical spin densities for radical cations of photosynthetic pigment models
Denis Artiukhin, Germany

PO1-171 Benchmarking structures and vibrational frequencies from subsystem DFT
Kevin Klahr, Germany

PO1-172 Optimization of optical properties: Inverse Design of dye-sensitized solar cells
Chencheng Fan, Germany

PO1-173 Benchmarking of semi-empirical QM/MM methods for proton transfers between biomacromolecules and aqueous solvent
Henning Henschel, Finland

PO1-174 Fast estimation of the dynamic electron correlation energy using localized molecular orbitals
Lisa Götte, Germany

PO1-175 Linear response formalism for internally contracted multireference coupled cluster theory to evaluate second order properties
Pradipta Samanta, Germany

PO1-176 Quantitative determinations of photochemistry from first principles: photoluminescence efficiencies of phosphors for OLEDs
Daniel Escudero, France

PO1-177 Statistical calibration of parametric property models
Jonny Proppe, Switzerland

PO1-178 Reactivity of copper carbenoid toward insertion in O-H bonds. A Density Functional Theory Study
Rocio Durán, Chile

PO1-179 Hidden electrostatic basis of dynamic allostery in a PDZ domain
Amit Kumawat, India

PO1-180 Computer-aided molecular design and modeling of catalysts capable of convert N2 into ammonia
Luis Miguel Azofra, Saudi Arabia

PO1-181 Theoretical study on the redox reaction mechanism of quinone compounds in industrial processes
Moto Tarumi, Japan

PO1-182 Au charge and its role in WGS reaction on reduced gold-substituted Ce1-xO2(111) surfaces
Wen-Shyan Sheu, Taiwan, Republic of China

PO1-183 The fluctuating charge model for improving force field electrostatics
Pier Paolo Poier, Denmark

PO1-184 Insight into molecular reactivity and reaction mechanisms from reactive molecular dynamics simulations
Sebastian Brickel, Switzerland

PO1-185 Polypyridyl iron(II) complexes as promising photoredox catalysts. Theoretical calculation of excited state redox potentials
Enrique Manuel Arpa González, Spain

PO1-186 Fast and accurate geometry optimization of lanthanoid complexes with an extended tight binding method
Markus Bursch, Germany

PO1-187 Automated exploration of complex chemical reaction networks
Gregor Simm, Switzerland

PO1-188 H2 dissociation and surface oxygen vacancy formation on (111)-CeO2 surface: a periodic DFT approach
Olivier Matz, France

PO1-189 Reaction rate constants from system-specific, black-box force fields parametrized by quantum chemical data
Julien Steffen, Germany

PO1-190 ϖ-Conjugated Macrocycles with High Radical Character
María Eugenia Sandoval-Salinas, Spain

PO1-191 Ligand-field states of aqua complexes revisited with multireference calculations: importance of solvation effects
Mariusz Radon, Poland

PO1-192 Benzene probes in molecular dynamics simulations reveal novel binding sites for ligand design
Yaw Sing Tan, Singapore

PO1-193 Molecular quantum-dot cellular automata based on diboryl radical anions
Xingyong Wang, Australia

PO1-194 Computational insights into the gas phase heterogeneous CO_2 reduction via surface frustrated Lewis pairs
Kulbir Ghuman, Japan

PO1-195 A scalable explicitly correlated local coupled-cluster method with pair natural orbitals: PNO-LCCSD-F12
Qianli Ma, Germany

PO1-196 Phosphinidene chalcogenides: DFT modeling of monomer trapping, ring expansion and mixed ring systems
Juuso Valjus, Finland

PO1-197 QM/MM modeling of PoXeR: a light-driven inward proton pump with unidirectional rotary motion
María Del Carmen Marín Pérez, Italy

Poster Session 1 – Monday, 28 August 2017

supported by ACS Energy Letters

PO1-198 Reaction mechanisms of polycyclic aromatic hydrocarbons with oxygen: site and size effects
Özlem Yönder, Germany

PO1-199 Studying the redox properties of DNA with hybrid quantum/classical molecular dynamics simulations
Polydefkis Diamantis, Switzerland

PO1-200 Towards branching ratio control in hot photoassociation of Mg2 - theory, numerics and experiment
Daniel Reich, Germany

PO1-201 Missing states and irregularities in excited states manifold of 2,2'-bithiophene - basis set dependence study
Marcin Andrzejak, Poland

PO1-202 Computational study of the reaction mechanism of the SCR of NOx using copper(II)-zeolite catalyst SSZ-13
Julian Rudolph, Germany

PO1-203 Fast QM/MM Electronic coupling calculationq for charge transfers in proteins
Natacha Gillet, Germany

PO1-204 Solvent accessibility and ligand binding in copper nitrite reductases
Kakali Sen, United Kingdom

PO1-205 MetScore: site of metabolism prediction beyond CYP P450 enzymes
Andreas Göller, Germany

PO1-206 DFT investigation for a new route of the Prins-reaction
Rodolfo Fiorot, Brazil

PO1-207 Developing inhibitors of the enzyme "TRMT2A" for the treatment of PolyQ diseases
Michael Alois Margreiter, Germany

PO1-208 Mechanistic insights into trifluoromethylation of a planar aryl-NiII complex involving NiIII/CF3• and NiIV-CF3 intermediate species
Josep M. Luis, Spain

PO1-209 New aspects of the reactivity of rhenium tricarbonyl complexes towards activated alkynes through DFT calculations
M. Isabel Menéndez Rodríguez, Spain

PO1-210 In silico design of zero thermal expansion materials
Andreas Erlebach, Germany

PO1-211 Structure over energy: an alternative approach for low-cost methods in crystal structure prediction
Luc LeBlanc, Canada

PO1-212 A kinetic model for singlet oxygen photosensitization
Shuming Bai, France

PO1-213 The role of acceptor-donor capacity in amide and imide dimerization. A theoretical-experimental study
Wilmer Vallejo, Mexico

PO1-214 Molecular dynamics study of lignin degradation under high pressure and temperature
ChinHui Yu, Taiwan, Republic of China

PO1-215 Excited state gradients in polarizable QM/MM models: an induced dipole formulation
Maximilian Menger, Austria

PO1-216 Computational insights into induction period of ethylene polymerization by the CrOx/SiO2 (Phillips) catalyst
Maciej Gierada, Poland

PO1-217 Theoretical studies on the cobalt(III)-based catalysts for CO_2/epoxide copolymerization
Monika Srebro-Hooper, Poland

PO1-218 An algorithm to locate optimal bond breaking points on potential energy surfaces for mechanochemical reactions
Jordi Ribas, Spain

PO1-219 A stochastic approach to thermal density functional theory
Yael Cytter, Israel

PO1-220 Comparing non-empirical DFT tuning procedures as a starting point for G0W0
Juliana Bois, Germany

PO1-221 Comparing anharmonic ab initio methods: Determining IR spectra of N2O5 + X- (X-=Cl-, Br-, I-)
Laura McCaslin, Israel

PO1-222 Accurate embedding based on potential reconstruction: top-down vs. Bottom-up
David Schnieders, Germany

PO1-223 The global reaction route map DB and QM-based conformational search
Hiroko Satoh, Japan

PO1-224 Large-scale first-principles GW+Bethe-salpeter simulations targeting 200 atom systems
Yoshifumi Noguchi, Japan

PO1-225 Implementation of divide-and-conquer density-functional tight-binding method for large-scale quantum mechanical molecular dynamics simulations
Yoshifumi Nishimura, Japan

Poster Session 1 – Monday, 28 August 2017

supported by ACS Energy Letters

PO1-226 Electronic structure properties of [n]Cyclacenes investigated by semi-empirical and wave function methods
Stefano Battaglia, France

PO1-227 Nonadiabatic simulations of carbon monoxide photodissociation in H64Q neuroglobin
Jakub Rydzewski, Poland

PO1-228 Difference of electron chirality between enantiomers as a possible solution to homochirality in Nature
Masato Senami, Japan

PO1-229 Heme vs. siroheme models of the sulfite reductase active site
Adrian Branzanic, Romania

PO1-230 Improved GBSA force field with modified CMAP and non-bonded interactions
Haiping Zhang, Singapore

PO1-231 Photochemistry of acrylic acid: semiempirical and Ab initio molecular dynamics vs. experiment
Dorit Shemesh, Israel

PO1-232 Combined quantum chemical calculations and QSPR on olefin polymerization using ansa-zirconocene for designing new catalysts
Vudhichai Parasuk, Thailand

PO1-233 Theoretical analysis on ion conduction in superconcentrated electrolyte solution for Na-ion battery
Masaki Okoshi, Japan

PO1-234 Decomposition of intermolecular interaction energies in the DLPNO-CCSD(T) framework. Theory and applications in homogenous catalysis
Giovanni Bistoni, Germany

PO1-235 Interpreting the hydrolysis/transglycosylation partition in a β-glucosidase using constant pH molecular dynamics
Inacrist Geronimo, Sweden

PO1-236 Calculation by QM of UV spectra of short-lived intermediates of OsCl62- in aqueous solutions
Marina Rogozina, Russian Federation

PO1-237 Activation Strain Model to understand oxidative addition of carbon-carbon bonds to Gold(I) complexes
Eric Daiann Sosa Carrizo, France

PO1-238 Sigma-hole carbon-bonding interactions in carbon-carbon double bonds: an unnoticed contact
David Quiñonero, Spain

PO1-239 Atom types introduction and RMSD-based selection for drug metabolites collision cross section calculation using MOBCAL
Dmytro Ivashchenko, Portugal

PO1-240 Uncommon molecular insertion complexes: non-dipoles and dipoles inside of dipoles
Fedor Naumkin, Canada

PO1-241 Tri-coordinated oxygen at the surface of graphene oxide (GO)
Tapas Kar, United States

PO1-242 Mechanistic Insight into imidazopyrazinone bioluminescence by TD-DFT calculations
Luís Pinto da Silva, Portugal

PO1-243 Perturbative Monte Carlo simulations - a hybrid QM/MM approach
Jonas Feldt, Germany

PO1-244 Structures and properties of silicon-doped boron clusters BnSi, with n = 15-24, and their anions
Thi Tuyet Mai Dang, Belgium

PO1-245 Spectroscopic properties of the redox-active tyrosine-D in photosystem II
Abhishek Sirohiwal, Germany

PO1-246 Evaluation of heats of formation of giant fullerenes using density functional tight binding
Simone Waite, Australia

PO1-247 Theoretical study on the properties of fac-Ir(ppy)3 and its derivatives
Yoshiki Natori, Japan

PO1-248 Investigating the interactions of novel anti-cancer therapeutics with DNA using computational modelling and spectroscopic techniques
Eunice Gwee, Australia

PO1-249 Electron fate and mutational robustness in the mechanism of (6-4) photolyase-mediated DNA repair
Hisham Dokainish, Japan

PO1-250 Computational Study of MEA adsorption on hydroxylated Cr_2O_3 surfaces
Theo De Bruin, France

PO1-251 Empirical force fields for simulating proton transfers: molecular dynamics and spectroscopy
Zhen-Hao Xu, Switzerland

PO1-252 Quantum chemical modelling of magnetic anisotropy and exchange interactions in lanthanide systems with 4fn5dm configurations
Akseli Mansikkamäki, Finland

Poster Session 1 – Monday, 28 August 2017

supported by ACS Energy Letters

PO1-253 Potential energy surface interpolation with neural networks for instanton rate calculations
April Cooper, Germany

PO1-254 Electronic properties and reorganization energies of the metal-metal-to-ligand charge transfer transition in Pt(II) complexes
Wei-Chih Chen, Taiwan, Republic of China

PO1-255 Calculation of reaction rate constants via instanton theory in the microcanonical ensemble
Andreas Löhle, Germany

PO1-256 DFT+D calculations of non-binding interactions of oligopyrrole aggregates doped with heptafluorotantalate (V) ions
Felipe Giraldo Nohra, Germany

PO1-257 The influence of chemical change on protein dynamics: a case study with pyruvate formate-lyase
Marko Hanževački, Croatia

PO1-258 Energies of molecular crystals from many body expansion combined with frozen density embedding
Daniel Schmitt-Monreal, Germany

PO1-259 Assessment of density functionals for computing thermodynamic properties of lanthanide complexes
Carine Clavaguera, France

PO1-260 Azobenzene photoisomerization in the strong coupling regime
Jacopo Fregoni, Italy

PO1-261 Interpolation of potential energy surfaces using gaussian process regression
Alexander Denzel, Germany

PO1-262 ϖ Electron Effects Control Diels-Alder Regioselectivity to Empty Fullerenes
Paula Pla, Spain

PO1-263 Application of the Bethe-Salpeter Equation to cationic dyes and n-ϖ* chromogens
Cloé Azarias, France

PO1-264 Flexible water docking and virtual screening using PLANTS combined with tuned water selection criteria
Xiao Hu, Italy

PO1-265 Theoretical investigation of Herzberg-Teller effects in resonance Raman spectra
Julien Guthmuller, Poland

PO1-266 Automated analysis of exchange pathways in spin-coupled systems
Torben Steenbock, Germany

PO1-267 New materials designed for absorption of non-steroidal antiinflammatory drugs
Anna Kaczmarek-Kedziera, Poland

PO1-268 Two-component relativistic density functional theory based on infinite-order Douglas-Kroll-Hess method
Yasuhiro Ikabata, Japan

PO1-269 Phosphorescent nechanism of arylboronic esters at room temperature
Qi Wang, Japan

PO1-270 A coupled state-averaged second-order MCSCF solver with fast convergence
David Amos Kreplin, Germany

PO1-271 Critical analysis of embedding schemes for QM/MM calculations in condensed phase
Martin Werner, Germany

PO1-272 Towards physical interpretation of the substituent effect
Halina Szatylowicz, Poland

PO1-273 Quest for PbII hydrides: when theory guides experiment
Jan Vícha, Czech Republic

PO1-274 Molecular dynamics study of the thermoresponsive polymer: poly(N-n-propylacrylamide) (PNnPAm)
Tiago Espinosa de Oliveira, France

PO1-275 The role of holes in borophenes, an ab-initio study of structural stability on Ag(111) surface
Naiwrit Karmodak, India

PO1-276 Nonlinear optical properties in helical molecules with pancake bonding
Shota Takamuku, Japan

PO1-277 ScSi2-/0 AND TiGe2-/0: electronic structures and insights into anion photoelectron spectra
Le Nhan Pham, Viet Nam

PO1-278 Stabilization of B-B triple bond in a metallaborocycle: contrast between boron and carbon analogs
Sagar Ghorai, India

PO1-279 Coupled electron-nuclear dynamics: a comparison of methods and dimensionality
Thomas Schnappinger, Germany

PO1-280 Reaction-prediction scheme based on quantum chemical information and machine learning
Mikito Fujinami, Japan

PO1-281 From structure to electronic properties of poly[methyl(phenyl)silylene] with DFT approach
Barbora Hanulikova, Czech Republic

Poster Session 1 – Monday, 28 August 2017

supported by ACS Energy Letters

PO1-282 [SbnAunSbn]m (n=4,5,6; m=-2, -1,-2) sandwich complexes as host of elements from groups I and II
Rafael Grande Aztatzi, Spain

PO1-283 Energetics of ion binding of the Na+/H+ antiporter MjNhaP1
Judith Warnau, Germany

PO1-284 Embedded multireference coupled cluster theory
David Coughtrie, Germany

PO1-285 Computational study of biologically active naphthylisoquinoline alkaloids: an overview of obtained results
Liliana Mammino, South Africa

PO1-286 Modern coupled cluster approaches for the spin-state energetics of carbenes
Reza Ghafarian Shirazi, Germany

PO1-287 Modelling the electronic states of polyphenylene-ethynylenes
Emmeline Ho, France

PO1-288 Relativistic calculations for identifying new chemical species at ultra-trace concentrations: AtO(OH)2- and IAtBr- revealed
Remi Maurice, France

PO1-289 Potential energy surfaces for dissociative collisions of atmospheric molecules
Yuliya Paukku, United States

PO1-290 Computational approach to organic reactions mechanisms in ionic liquids
Christian Silvio Pomelli, Italy

PO1-291 DFT mechanism of chelating ruthenium catalysts new for ring opening metathesis polymerization (ROMP)
Katerine Paredes, Chile

PO1-292 Towards an accurate first-principles description of excited states in dielectric wnvironments: the versatile ADC(0-3)/SS-PCM approach
Jan-Michael Mewes, New Zealand

PO1-293 Thermochemical properties of BaXO3 (X=Mn, Zr, Ce) perovskite materials using first principles phonon calculations
Krishna Kamol Ghose, Australia

PO1-294 Behavior of finite uniform electron gases at high and low density
Marat Sibaev, Australia

PO1-295 Is a post-self-consistent-field addition of the non-local correlation kernel in van-der-Waals density functionals sufficient?
Asim Najibi, Australia

PO1-296 Exciton transference in natural and hypothetical bacteriochlorophyll arrangements. Is singlet fission a possible photosynthetic mechanism?
Joaquin Barroso, Mexico

PO1-297 An efficient method for calculating effective core potential integrals
Simon McKenzie, Australia

PO1-298 Evaluation of aromaticity based on magnetically induced current using the GIMIC method for open-shell molecules
Takanori Nagami, Japan

PO1-299 Chiral glycine methyl ester - chirality transfer in matrix-isolation vibrational circular dichroism (MI-VCD) spectroscopy
Dennis Gerbig, Germany

PO1-300 Surface effects on vacancy diffusion in titanate perovskites ATiO3 (A = Sr2+, Ba2+, Ca2+)
Joshua Brown, Australia

PO1-301 Short-range spin-dependent interaction energies between chiral molecules
Steffen M. Giesen, Germany

PO1-302 Concerted proton transfer in mixed acid-water clusters: [(HCl)(H2O)]2 and [(HF)(H2O)]4
Itay Zakay, Israel

PO1-303 Insights into the formation of catalytically active metal-substituted polyoxometalates in the presence of proteins
Dragan Conic, Belgium

PO1-304 Conformational analysis and accurate prediction of molecular properties for highly flexible chiral natural products
Muhammad Ali Hashmi, New Zealand

PO1-305 Density-functional tight-binding molecular dynamics simulations of proton diffusion in the bulk ices and liquid water
Aditya Wibawa Sakti, Japan

PO1-306 Accurate prediction of one-electron reduction potentials of transition metal complexes
Daniel Bim, Czech Republic

PO1-307 Concentration dependence of sound velocity in water and methanol mixtures using molecular-dynamics simulation
Masafumi Yamasaki, Japan

Poster Session 2 – Tuesday, 29 August 2017

supported by The Journal of Physical Chemistry

PO2-1 A new approach for the balanced description of dynamic correlation and spin-dependent relativistic effects
Lucas Lang, Germany

PO2-2 Cooperative effect in water cluster
Imre Bakó, Hungary

PO2-3 Exploring and pushing the limits of ansa-aminoborane reactivity
Imre Pápai, Hungary

PO2-4 Intramolecular singlet fission: insights from multireference perturbation theory and quantum dynamical simulations
Pedro B. Coto, Germany

PO2-5 Charge-transfer states in donor-acceptor pairs connected by the salt bridge
Ivana Antol, Croatia

PO2-6 Non-adiabatic dynamics at metallic surfaces: revisiting the NO/Au(111) puzzle
Tobias Serwatka, Germany

PO2-7 Analysis of electron correlation effects in strongly correlated systems (N2/N2+)
Christian Stemmle, Germany

PO2-8 Theoretical study on exchange interaction between f and ϖ electrons in Tb(III)-phthalocyanine double-decker complex
Yasutaka Kitagawa, Japan

PO2-9 Fitted potential energy surfaces in non-redundant, translationally and rotationally invariant coordinate systems
Sean McConnell, Germany

PO2-10 Oxygen reduction reaction on a defective ZrO_2 surface
Yoshiyuki Yamamoto, Japan

PO2-11 Computing bulk phase infrared, raman, VCD, and ROA spectra from ab initio molecular dynamics
Martin Brehm, Germany

PO2-12 A theoretical mechanistic study on the reaction of a rhenium hydroxo complex toward methyl propiolate
Ramón López, Spain

PO2-13 A catalytic oxidation mechanism for the first C-H bond of organic molecules by MnO_2
Kai Huwig, Germany

PO2-14 Ionization potentials, electron affinities, and photoelectron spectra: comparing various DFT and GW methods
Lukas Gallandi, Germany

PO2-15 Dynamic aolvent wffects treated with a quantum/classical TDSCF approach
Martin Peschel, Germany

PO2-16 QM/MM study of an atom tunneling in the hydroxylation process of taurine/αketoglutarate dioxygenase (TauD)
Sonia Álvarez Barcia, Germany

PO2-17 Replacing coarse-grained ligand on binding site by all-atom model
Tenfu Suzumura, Japan

PO2-18 Theoretical investigation of organic ligands radiation stability
Artem Mitrofanov, Russian Federation

PO2-19 Influence of atom-tunneling and ice surfaces on the reaction rates of interstellar water formation
Jan Meisner, Germany

PO2-20 A quantum chemical definition of electron-nucleus correlation energy
Patrick Cassam-Chenaï, France

PO2-21 The incremental EOM-CCSD method and study of UV-Vis spectra in ThDP-dependent enzymes
Mirko Paulikat, Germany

PO2-22 Dynamic electron correlation for compact non-orthogonal orbital expansions of large active spaces
Sven Kähler, Denmark

PO2-23 Experimental and computational investigations on the enantioselective alkynylation of α-ketoesters via copper catalysis
Martin Christoph Schwarzer, Japan

PO2-24 Ultracold chemistry: theory of photoassociation processes of alkali metal clusters
Jan Schnabel, Germany

PO2-25 Analysis of energy contributions to environmental effects on excited states
Heiner Schröder, Germany

PO2-26 Adsorption of CO_2 and methane onto olivine surfaces in Mars conditions
C. Ignacio Sainz-Diaz, Spain

PO2-27 Modeling of nonlinear optical response
Carolin Hühn, Germany

PO2-28 Bond indicators from relativistic and multiconfigurational calculations: application to astatine species
Cecilia Gomez Pech, France

PO2-29 Tensor decomposition methods for correlated electron pairs
Airi Kawasaki, Japan

Poster Session 2 – Tuesday, 29 August 2017

supported by The Journal of Physical Chemistry

PO2-30 Analytical stress tensor with density fitting and continuous fast multipole methods
Martin Becker, Germany

PO2-31 Computational studies into the mechanism of cobalt-catalysed carboxylate-assisted C-H activation
Samuel Neale, United Kingdom

PO2-32 On the origin of stereoselectivity in FLP-catalyzed asymmetric hydrogenation of imines
Andrea Hamza, Hungary

PO2-33 Theoretical investigation of a Cloke-Wilson rearrangement of VCP with a photoactive Fe-nitrosyl-catalyst
Florian Bauer, Germany

PO2-34 Quantum chemical conformational analyses unveil conformational flexibility of physiological (l-histidinato)(l-threoninato)copper(II) in aqueous solution
Jasmina Sabolovic, Croatia

PO2-35 Time-dependent quantum description of double core hole states formation in carbon monoxide
Solene Oberli, France

PO2-36 Characterization of PTCDA thin films and the electronic character: the dimer picture and beyond
Daniel Bellinger, Germany

PO2-37 Broken-symmetry solutions and magnetic exchange couplings from subsystem DFT
Anja Massolle, Germany

PO2-38 Efficient approaches for multidimensional quantum dynamics: dynamical pruning in phase, position and configuration space
Henrik R. Larsson, Germany

PO2-39 Simulation of glycine precusor formation in the interstellar medium
Max Markmeyer, Germany

PO2-40 Proton loading site in cytochrome c oxidase
Jovan Dragelj, Germany

PO2-41 TDDFT-based protocol with local hybrid functionals for the screening of potential singlet fission chromophores
Robin Grotjahn, Germany

PO2-42 Protonation effects on the multi-photoelectron storage capacity of a series of novel black absorbers
Philipp Traber, Germany

PO2-43 Metastability of the low-lying electronic states of CBr2+: A CASSCF/MRCI study
Tiago Alves, Brazil

PO2-44 Treatment of molecular Feshbach resonances in equation-of-motion coupled-cluster theory
Thomas Jagau, Germany

PO2-45 AB initio investigation of trans-[RuCl(NO)(py)4]2+ photochemistry
Francesco Talotta, France

PO2-46 A rising star: Truxene as a promising hole transport material in perovskite solar cells
Kun-Han Lin, Switzerland

PO2-47 Analytical first derivatives for DLPNO-MP2
Peter Pinski, Germany

PO2-48 Formation of cyclic and acyclic oligosilanes from SiCl2 - A DFT assessment
Lioba Meyer, Germany

PO2-49 Multiconfigurational ab initio and DFT study of metal-metal bonded diruthenium mixed valence complexes Luís
Henrique Ferreira de Moraes, Brazil

PO2-50 Nonadiabatic dynamics of intramolecular singlet fission in covalently linked pentacene dimers
Seelam Rajagopala Reddy, Germany

PO2-51 Recent developments on local hybrid functionals
Toni Mike Maier, Germany

PO2-52 Lessons from the spin-polarization/spin-contamination dilemma of transition-metal hyperfine couplings for the construction of new functionals
Caspar Jonas Schattenberg, Germany

PO2-53 Reactive intermediates involving group IV and VI metal centers. Joint UV-PES - DFT studies
Jean-Marc Sotiropoulos, France

PO2-54 Calculating protein-ligand binding affinities with the quantum-mechanical GFN-xTB method
Katja Ostermeir, Germany

PO2-55 Explicit description of solvent is important to predict the electronic properties of phthalocyanines derivatives?
Felipe Cesar Torres Antonio, Brazil

PO2-56 Oligothiophene molecules on a metal substrate: electronic response to supramolecular packing
Laura Katharina Scarbath-Evers, Germany

PO2-57 A materials genome approach to catalysis: transforming waste CO2 to value-added products like methanol
Andrew Harris, United States

Poster Session 2 – Tuesday, 29 August 2017

supported by The Journal of Physical Chemistry

PO2-58 Insights of the photoredox catalysis from a computational point of view
Miquel Torrent Sucarrat, Spain

PO2-59 Effects of relativity on the structure of metal complexed crown ethers
Meagan Oakley, Canada

PO2-60 Molecular hydrogen formation onto PAH surface analyzed by reaction force and activation strain model
César Barrales-Martínez, Chile

PO2-61 Atomic force spectroscopy of streptomycin binding aptamer: an out-of-equilibrium molecular dynamics study
Paulo Netz, Brazil

PO2-62 Modeling of oligosaccharides within glycoproteins from free-energy landscapes
Aysegul Turupcu, Austria

PO2-63 Superatomic states in nickel clusters: revising the prospects for transition metal based superatoms
James Gilmour, New Zealand

PO2-64 Towards a theoretical description of solidstate materials made from superatoms and fullerenes as building blocks
Lukas Hammerschmidt, New Zealand

PO2-65 Electronic properties of DNA: description of weak interactions and reactivity of TATA box models
Jorge Gutiérrez-Flores, Mexico

PO2-66 Hydrogen adsorption and spillover mechanisms on metal-doped carbon nanohorn: Insights from DFT calculations
Chompoonut Rungnim, Thailand

PO2-67 Using frontier molecular orbital analysis for prediction of regioselectivity of 1,4,5-trisubstituted 1,2,3-triazoles synthesis
Waraporn Parasuk, Thailand

PO2-68 Density-functional tight-binding parameterization for metal-orgranic frameworks
Chien-Pin Chou, Japan

PO2-69 Decomposing the origin of Hofmeister effects
Kasimir Gregory, Australia

PO2-70 Configuration interaction singles and doubles using exact exchange kohn sham orbital in real-space grid method
Jaechang Lim, Republic of Korea

PO2-71 Base catalyst role on the silylation of secondary alcohols
Marta Marin-Luna, Germany

PO2-72 Electronic excitation spectra calculation of large systems with a tight-binding based simplified Tamm-Dancoff approximation (sTDA-xTB)
Jakob Seibert, Germany

PO2-73 Molecular dynamics simulations of different prion variants
Ayşenaz Tavşanlı, Turkey

PO2-74 An additive QM/MM approach for the calculation of molecular crystals
Thorsten Teuteberg, Germany

PO2-75 Electronic couplings for molecular charge transfer: the case of antiferromagnetically coupled systems
Adam Kubas, Poland

PO2-76 Fulvenes as a new class of triplet ground state biradicals stabilized by Baird aromaticity
Kjell Jorner, Sweden

PO2-77 Partial Hessian techniques in vibrational circular dichroism
Tiago Teodoro, Netherlands

PO2-78 Selenium in GPx biochemistry: Insights from DFT studies on model chalcogenides
Marco Bortoli, Italy

PO2-79 Linear-scaling generation of potential energy surfaces for anharmonic vibrational spectra calculations
Carolin König, Sweden

PO2-80 Hybrid QM/MM molecular dynamics with AMOEBA polarizable embedding
Daniele Loco, Italy

PO2-81 A mechanistic exploration of the plasma formation of perchlorosilanes
Julia I. Schweizer, Germany

PO2-82 QM/MM study of the reaction mechanism of the box H/ACA pseudouridine synthase catalysed uridine isomerisation
Dóra Judit Kiss, Hungary

PO2-83 vdW-DF+U description of solid oxygen
Shusuke Kasamatsu, Japan

PO2-84 Bonding of carbonyl groups to the dipentalene dititanium system relating to products from CO_2 activation
Luana-Flavia Radu, Romania

PO2-85 Big data analysis of the NDDO approximation to ab initio molecular electronic integrals
Xin Wu, Germany

Poster Session 2 – Tuesday, 29 August 2017

supported by The Journal of Physical Chemistry

PO2-86 Analytical nuclear excited-state gradients using frozen-density embedding to investigate molecular response in an explicit environment
Johannes Heuser, Germany

PO2-87 Semiempirical quantum mechanical scoring functions for computer aided drug design
Jindrich Fanfrlik, Czech Republic

PO2-88 Simulating osmotic equilibria: a new tool to calculate activities in concentrated solution
Michael Bley, France

PO2-89 A perturbation-based Super-CI approach for the orbital optimization of a CASSCF wave function
Christian Kollmar, Germany

PO2-90 Baird´s rule under the umbrella of Clar's rule: a means for tuning triplet state energies
Rabia Ayub, Sweden

PO2-91 Allosteric control of the DNA-RNA translocation in telomerase
Aydin Ozmaldar, Turkey

PO2-92 The automated topology builder (ATB): a big data approach to empirical force field parameterisation
Martin Stroet, Australia

PO2-93 Mechanistic investigation of CO oxidation on a single gold atom deposited on MgO(001) surfaces
Kai Töpfer, Germany

PO2-94 Hybrid functionals approach of the structural, electronic and dynamical properties of semiconductors for photovoltaic applications
Fabien Lafond, France

PO2-95 Excited-state dynamics of a eumelanin building block: photoprotection or photodamage?
Juan Jose Nogueira Perez, Austria

PO2-96 Trends in the Au adsorption energy on oxide surfaces: a DFT study
Sergio Tosoni, Italy

PO2-97 QM:QM calculations on molecular crystals
A. Daniel Boese, Austria

PO2-98 Raman technique and density functional theory - the "R"&"D" in research and development of antibiotics
Ana Maria Raluca Gherman, Romania

PO2-99 Thermal conductivity of group 4 layered transition metal disulfides: a first-principles study
Nina Glebko, Finland

PO2-100 Electronic excitations of 6-Hydroxyindole-based BODIPY fluorophore: polarization propagator approach and explicit solvation
Anna Skitnevskaya, Russian Federation

PO2-101 Photoreactivity of adenine and cytosine with water molecules via electron-driven proton-transfer processes
Xiuxiu Wu, Germany

PO2-102 Low-lying electronic terms of diatomic molecules AB (A = Sc - Ni, B = Cu/Ag/Au)
Davood Alizadeh Sanati, Germany

PO2-103 Terminal electron-proton transfer dynamics coupled to quinone reduction in respiratory complex I
Ana Patricia Gamiz Hernandez, Germany

PO2-104 Toward a W4-F12 approach: Can explicitly correlated and orbital-based ab initio CCSD(T) limits be reconciled?
Nitai Sylvetsky, Israel

PO2-105 Investigation of the gas-phase hydrolysis of organocuprates by quantum chemical and master equation calculations
Thomas Auth, Germany

PO2-106 Effect of dipole moment on formation of trap states in CdS nanocrystals
Anuar Aldongarov, Kazakhstan

PO2-107 Spherical or prismatic: a computational study of metal-doped ten-vertex lead clusters
Matei-Maria Uta, Romania

PO2-108 Revealing multi-centre bonding contributions from an electron density perspective using FALDI
Daniel van Niekerk, South Africa

PO2-109 How to quantify charge transfer character of excited states in transition metal complexes
Sebastian Mai, Austria

PO2-110 Performance of GGA and hybrid density functionals in calculation of lattice thermal conductivity of Cu_2O
Jarno Linnera, Finland

PO2-111 Conformational scan across reaction path may give us fake transition states with low energy
Andrus Metsala, Estonia

PO2-112 Inevitability of ab initio calculations in determining large magnetic anisotropy
Arup Sarkar, India

PO2-113 It´s getting hot: temperature-dependent Wigner sampling
Patrick Zobel, Austria

Poster Session 2 – Tuesday, 29 August 2017

supported by The Journal of Physical Chemistry

PO2-114 Conformational Dependence of Partial Charges Derived from Quantum-Mechanical Calculations
Jagna Witek, Switzerland

PO2-115 A general intermolecular force field based on tight-binding quantum chemical calculations (xTB-IFF)
Jana Pisarek, Germany

PO2-116 On the controversial stereoselectivity models of organocatalyzed michael additions of aldehydes to nitroalkenes
Tamás Földes, Hungary

PO2-117 A three-state model for the Photo-Fries rearrangement
Josene Maria Toldo, Brazil

PO2-118 Investigation of perfluorinated compound-binding to human hepatocyte nuclear factor (HNF4α)
Esra Boz, Germany

PO2-119 The role of conical intersections in aggregation induced emission
Michael Dommett, United Kingdom

PO2-120 Carbocatalysis: a computational insight into the metal-free oxidation of ethylbenzene by carbonanotubes
Tainah Dorina Marforio, Italy

PO2-121 Dynamical studies on the photodissociation of diphenylmethyl bromide
Franziska Schüppel, Germany

PO2-122 Predicting selectivity for covalent inhibitors from QM/MM, Docking and MD - What is possible?
Thien Anh Le, Germany

PO2-123 Systematic calibration of a transferable polarizable force field parameter set
Daan Geerke, Netherlands

PO2-124 Excited states of molecular aggregates predicted by a model Hamiltonian tuned toward high-level quantum-chemical calculations
Sofia Canola, Italy

PO2-125 The effect of a mobile solvent environment on quantum control of chemical reactions
Daniel Keefer, Germany

PO2-127 Influence of neighboring nucleobases on the photostability of uracil: quantum dynamics in explicit biological environments
Sebastian Reiter, Germany

PO2-128 Mimicking metalloenzymes with cyclodextrins: what can we learn from modeling?
Etienne Derat, France

PO2-129 Förster resonance energy transfer in a noval ligth-harvesting polymer investigated state-of-the-art multiconfigurational methodes and TDDFT
Michael Siegmann, Germany

PO2-130 Canonical formats in chemical kinetics and slow manifold approximation
Alessandro Ceccato, Italy

PO2-131 Catalytic mechanism and molecular engineering of quinolone biosynthesis in dioxygenase AsqJ
Sophie Mader, Germany

PO2-132 The polarizable density embedding coupled cluster method
Dalibor Hršak, Denmark

PO2-133 Hydrodesulfurization mechanisms of dibenzothiophene molecules catalyzed by CoMoS catalysts: a DFT study
Alexandre Samuel Dumon, France

PO2-134 Computational bioinorganic chemistry of [Cu2O2]2+ complexes: selective hydroxylation of aliphatic C-H bonds
Moritz Förster, Germany

PO2-135 Hydrogen evolution mechanisms of Bis-terpyridyl cobalt catalysts: a ligand-based vs. a metal-based pathway
Tanya K. Todorova, France

PO2-136 Bringing order to unordered compounds: The phase system Li-Ag-Ge
Jasmin Dums, Germany

PO2-137 An accurate ab-initio parametrization of density functional dispersion coerrection (DFT-D4) for the 86 elements H-Rn
Eike Caldeweyher, Germany

PO2-138 GW based methods in quantum chemistry
Christof Holzer, Germany

PO2-139 Density functional studies of tetrapyrroles on Ag(111)
Jan-Niclas Luy, Germany

PO2-140 Detailed quantitative and visual analysis methods for electronic excitation processes
Felix Plasser, Austria

PO2-141 Quantification and theoretical analysis of the electrophilicities of michael acceptors
Harish Harish, Germany

PO2-142 Quantum molecular trajectory: the road to quantum description of molecular motions
Francesco Avanzini, Italy

Poster Session 2 – Tuesday, 29 August 2017

supported by The Journal of Physical Chemistry

PO2-143 Ab initio prediction of co-adsorption of gases by GCMC simulations on a lattice of sites
Arpan Kundu, Germany

PO2-144 DFT investigations into the dehydropolymerisation of amine-boranes using [(tBuXantphos)Rh(H)]
Nicholas Beattie, United Kingdom

PO2-145 Conformational analyses of bis(L-asparaginato)copper(II) in the gas phase and in aqueous solution
Marijana Marković, Croatia

PO2-146 Electron-driven solvent effects alter photochemistry of 2-thiocytosine
Mikołaj Janicki, Poland

PO2-147 A down-folded effective Hamiltonian combining many-body perturbation theory with configuration interaction
Marc Dvorak, Finland

PO2-148 Bonding situation in C2E2 (E = N, P, As, Sb, Bi) ligand stabilized complexes
Diego Andrada, Germany

PO2-149 Aggregation of MB in water and water/urea mixtures: the role of solute polarization
Cleiton Maciel, Brazil

PO2-150 Multi-level QM:QM adsorption studies within MonaLisa program
Maristella Alessio, Germany

PO2-151 Excited state hydroxide ion transfer in aqueous media: Ab-Initio MD simulation of a bifunctional chromophore
Felix Hoffmann, Germany

PO2-152 Computational study of DNAzyme 9DB1: prediction of the pre-catalytical conformation and the reaction mechanism
Juan Aranda Moratalla, Spain

PO2-153 Random phase approximation for periodic systems employing direct coulomb lattice summation
Martin Grundei, Germany

PO2-154 Investigation of electron transfer rates in a Ru-Pd molecular photocatalyst
Magdalena Staniszewska, Poland

PO2-155 Computational study of halloysite as a tubular nanocarrier to control drug release
Ana Borrego-Sánchez, Spain

PO2-156 Frozen virtual natural orbitals for coupled cluster properties
Ashutosh Kumar, United States

PO2-157 Quantum chemical studies of a hemithioindigo-based photodriven molecular motor
Florian Rott, Germany

PO2-158 Electronic excited states of organic molecules adsorbed on Cu(100)
Fernando Aguilar-Galindo, Spain

PO2-159 Homogeneous volcano plots: in search of new metal-pincer complexes for the hydrogenation of carbon dioxide
Boodsarin Sawatlon, Switzerland

PO2-160 Keto-enol tautomerization on the bioluminescence emitter in fireflies
Romain Berraud-Pache, France

PO2-161 Modelling environmental effects for excitations in molecular crystals
Miguel Rivera, United Kingdom

PO2-162 Algebraic diagrammatic construction with coupled-cluster amplitudes: improved static dipole polarizabilities
Manuel Hodecker, Germany

PO2-163 Modeling the modulation of emission behavior in E/Z isomers of diphenyldipyrroethene
Laura Le Bras, France

PO2-164 Watson-Crick ↔ Hoogsteen transitions in duplex DNA: a systematic MD study
Hansel Gomez, Spain

PO2-165 Testing the effectiveness of the isoelectronic substitution principle through the transformation of aromatic osmathiophene derivates
Rafael Islas, Chile

PO2-166 Modulation of energetic landscape under different electron conducting regimes in bacterial nanowires
Alexandre Hernandes Barrozo, United States

PO2-167 On the mechanism of frustrated Lewis pair catalysed hydrogenation of carbonyl compounds
Shubhajit Das, India

PO2-168 Simulation of structure and electronic spectra of 1,3,4-oxadiazole chromophores
Juozas Sulskus, Lithuania

PO2-169 A direct spin-orbit CAS-CI program designed for molecule magnets
Karin Fink, Germany

PO2-170 A lower scaling coupled cluster method for excited states
Achintya Kumar Dutta, Germany

PO2-171 QM modeling of organic-inorganic hybrid materials as heterogeneous catalysts for pharma industry
Marta Corno, Italy

Poster Session 2 – Tuesday, 29 August 2017

supported by The Journal of Physical Chemistry

PO2-172 Oxygen evolution reaction on pristine and nitrogen-doped carbon nanotubes
Garold Murdachaew, Finland

PO2-173 Deactivation of hazardous chemicals at oxide surfaces
Tobias Klöffel, Germany

PO2-174 Automated multi-configurational calculations
Christopher Stein, Switzerland

PO2-175 Photodissociation dynamics and spectroscopy in the presence of conical intersections
David Picconi, Germany

PO2-176 Absorption of graphene to metal (111) surfaces using the exchange-hole dipole moment model
Matthew Christian, Canada

PO2-177 Adiabatic variational theory for anisotropic atom-diatom collisions at very low temperatures
Mariusz Pawlak, Poland

PO2-178 Cation-ϖ interactions in CREBBP inhibition: an electrostatic model for small-molecule binding affinity and selectivity
Kiran Kumar, United Kingdom

PO2-179 A generalized empirical potential to describe halogen bonds
Lucas de Azevedo Santos, Brazil

PO2-180 The role of intramolecular interactions on the bioactive conformation of epinephrine
Daniela Rodrigues Silva, Brazil

PO2-181 Oganesson: rare gas or not? Monte-Carlo melting simulations of heavy and super-heavy group-18 elements
Paul Jerabek, New Zealand

PO2-182 Importance of local exact exchange potential in hybrid functionals for accurate excited states
Jaewook Kim, Republic of Korea

PO2-183 Non-adiabatic molecular dynamics simulations for elucidating high photoluminescence (PL) efficiency of dual chromophores material
Jiwon Moon, Republic of Korea

PO2-184 Phosphorescent lifetimes of perfluoro-substituted Iridium complexes as deep-blue OLED materials
Kiyull Yang, Republic of Korea

PO2-185 A theoretical study of the recognition of a neutralizing antibody to the HIV-1 envelope glycoprotein
Kaori Ueno-Noto, Japan

PO2-186 Comparison Se-Se bond in SeHCl···SeHCl and cyclic SeHCl···SeHCl···X (X = SHCl, ClCl, SeHCl, BrCl) complexes
Lingpeng Meng, China

PO2-187 Electrochemical properties of anatase-type TiO2 nanoparticles - a theoretical approach
Gergely Juhasz, Japan

PO2-188 Nature of MH…X bond in Cp2Mo(L)H …I-C≡C-R complexes
Xiaoyan Li, China

PO2-189 SMASH: massively parallel quantum chemistry program
Kazuya Ishimura, Japan

PO2-190 Theoretical approaches on isothermal crystallization behavior of β-nucleating agent filled glass fiber/polypropylene composites
Jong Sung Won, Republic of Korea

PO2-191 Relationship between open-shell character and third-order nonlinear optical properties in rectangular-shaped tetraradical model systems
Hiroshi Matsui, Japan

PO2-192 Modelling the LCST behaviour of tactic poly(PEGMA)
Brad Wells, Australia

PO2-193 Semiempirical OMx/MRCI methods: comprehensive benchmarks of electronically excited states and surface-hopping dynamics of a biomolecule
Deniz Tuna, Germany

PO2-194 Modulating charge-transfer between fluorescein-porphyrin-based chromophores and TiO2 in dye-sensitized solar cells
Gloria Cardenas-Jiron, Chile

PO2-195 TDDFT investigation of manipulation of the electronic and optical properties of phosphorus containing heteroacenes
Heehyun Baek, Republic of Korea

PO2-196 IQmol - the smart choice in molecular visualization software
Andrew Gilbert, United States

PO2-197 MDbox: a cloud-based repository for molecular dynamics simulations
Karmen Condic-Jurkic, Australia

PO2-198 Electronic properties of bilayer gallium
Dani Metin, New Zealand

Poster Session 2 – Tuesday, 29 August 2017

supported by The Journal of Physical Chemistry

PO2-199 Probing supramolecular self-assembly with molecular dynamics simulations
Michael Thomas, Australia

PO2-200 Computational results for the cobalt and platinum paired single-atom catalysis of the oxygen reduction reaction
Julia Melisande Fischer, Australia

PO2-201 La or Lb, that is the question! - quantum dynamical and semi-classical studies of pyrene
Matthias K. Roos, Germany

PO2-202 Energy transfer in Fenna-Matthews-Olson complex with a realistic all-atom interpolated potential model
Chang Woo Kim, Republic of Korea

PO2-203 Density functionals in the studies of dipole moment and polarizability of the spatially confined molecules
Marta Chołuj, Poland

PO2-204 Computational insight into Fe@C-catalyzed Fischer-Tropsch synthesis
Geraldine Cilpa-Karhu, Finland

PO2-205 Pseudo ϖ-hole Interactions vs ϖ-hole Interactions
Yanli Zeng, China

PO2-206 Consistent interpretation of coarse-grained peptide kinetics using Markov state models biased with external information
Joseph Rudzinski, Germany

PO2-207 How does Ga4L6 supramolecular cage help carbocation cyclizations?
Q. Nhu Nguyen, United States

PO2-208 Towards accurate description of weak and strong correlations via spin-projection
Takashi Tsuchimochi, Japan

PO2-209 On the use of Gaussian process regression in geometry optimizations
Gunnar Schmitz, Denmark

PO2-210 Anharmonic vibrational spectra from double incremental potential energy surfaces and dipole surfaces
Diana Madsen, Denmark

PO2-211 Simulating rare events with the adaptive multilevel splitting method
Laura Joana Silva Lopes, France

PO2-212 Catalyzed decomposition of Alkyl hydroperoxides to ketones - a mechanistic investigation
Marko Hermsen, Germany

PO2-213 cosmori-cc2: a polarizable continuum ri-cc2 method for calculation of vertical excitation energies and analytic gradients
Sarah Karbalaei Khani, Germany

PO2-214 The oxidative coupling of methane: first-principles micro-kinetic modeling
Matthias Baldofski, Germany

PO2-215 Accurate calculation of alkali metal peroxides and superoxides dissociation
Aleksandr Zaichenko, Germany

PO2-216 Light-triggered CO Release in novel manganese complexes : a quantum chemical investigation
Johannes Steinmetzer, Germa ny

PO2-217 Rational design of single molecule magnets
Matija Zlatar, Serbia

PO2-218 Theoretical study on analog of carbodicarbene: NBO and mechanism of addition reaction
Yusuke Kuroda, Japan

PO2-219 Towards understanding strong electron correlation in molecular complexes on surfaces
Marc Philipp Bahlke, Germany

PO2-220 Strong-scaling parallelization of ab initio calculations on massively parallel architectures
Jörg Kussmann, Germany

PO2-221 Full-dimensional excited-state intramolecular proton transfer dynamics of salicylic acid
Tim Raeker, Germany

PO2-222 New insights on aromatic pathways in porphyrinoids by calculations of magnetically induced currents
Heike Fliegl, Norway

PO2-223 Selective catalytic reduction of NO with NH_3 over Ru-doped CeO_2 investigated by DFT method
Chirawat Chitpakdee, Thailand

PO2-224 Structure optimization of temporary anions with CAP-EOM-CC methods using analytic gradients
Zsuzsanna Benda, Germany

PO2-225 Environmental effects on the UV-Vis spectra of chlorophyll in the LHCII protein complex
Souloke Sen, Netherlands

PO2-226 Theoretical analyses of solid electrolyte interphase film formation in secondary batteries via Red Moon method
Norio Takenaka, Japan

PO2-227 Bridging time scales with variationally enhanced sampling
Omar Valsson, Germany

Poster Session 2 – Tuesday, 29 August 2017

supported by The Journal of Physical Chemistry

PO2-228 Performance of range-separated hybrid functional with Krieger-Li-Iafrate potential for molecular excitation energies
Sungwoo Kang, Republic of Korea

PO2-229 Computational NMR spectroscopy for host-guest hemicarcerands
Abril C. Castro, Spain

PO2-230 When 2 is better than 1: variational Geminal theory
Stijn De Baerdemacker, Belgium

PO2-231 Computational insights into dispersion interactions in self-assembled supramolecular host-guest systems
Axel Wuttke, Germany

PO2-232 Macrocycle conformational sampling by DFT-D3/COSMO-RS methodology
Ondrej Gutten, Czech Republic

PO2-233 Modelling the reactions catalysed by coenzyme B12 dependent enzymes: Accuracy and cost-quality balance
Christian Wick, Croatia

PO2-234 Why do novel mo-alkylidene catalysts facilitate olefin metathesis in the presence of functional groups?
Maren Podewitz, Austria

PO2-235 Database of benchmark interaction energies mapping repulsive contacts in organic molecules
Vijay Madhav Miriyala, Czech Republic

PO2-236 Extended single-reference vibrational coupled cluster for the description of molecular double-well systems
Mads Bøttger Hansen, Denmark

PO2-237 Open-shell character from experimental and calculated bond lengths
Bodo Alexander Voigt, Germany

PO2-238 Chemical bonding and adsorption dynamics of cyclooctynes in the creation of organic/inorganic interfaces
Lisa Pecher, Germany

PO2-239 Exciton dynamics in Light Harvesting Complexes: From ab initio TDDFT calculation towards Open System models
Joaquim Jornet-Somoza, Spain

PO2-240 How to describe quantum interferences to separate nuclear spin isomers
Sandra Gomez Rodriguez, Austria

PO2-241 Theoretical investigation of silafulleranes with an endohedral guest
Josef H. Wender, Germany

PO2-242 First-order properties within MP2 using Cholesky decomposed density matrices and the resolution-of-the-identity approximation
Sigurd Vogler, Germany

PO2-243 Towards a roadmap of chemical space: using reaction networks to study catalysis
Johannes Margraf, Germany

PO2-244 Increased accuracy and reduced computational cost within the resolution-of-the-identity random phase approximation
Henry Schurkus, Germany

PO2-245 A local coupled cluster investigation of non-heme iron complexes
Milica Feldt, Belgium

PO2-246 Origin of regio- and stereoselectivity in Michael additions of pyrrolidine enamine derivatives
Tamara Husch, Switzerland

PO2-247 Two interacting molecules in a one-dimensional harmonic trap
Anna Dawid, Poland

PO2-248 Formation of deoxyribonucleotide in prebiotic conditions
Danijela Barić, Croatia

PO2-249 Chemically functionalized graphene derivatives for optoelectronic and chemical sensing applications
Lukas Eugen Marsoner Steinkasserer, Germany

PO2-250 Fast prediction of the specific conductivity of electrolytes from the molecular structure of the solvent
Rémi Bouteloup, France

PO2-251 Efficient calculation of electron-phonon coupling in molecular junctions
Michael Deffner, Germany

PO2-252 Mechanism of methyl transfer between methylcobalamin and A-cluster in acetyl-coenzyme A synthase (ACS). DFT calculations
Maria Jaworska, Poland

PO2-253 Lattice energies of molecular solids from fragment and periodic approaches
Jaroslav Hofierka, Czech Republic

PO2-254 Mechanistic investigations of electronic current dynamics through a single-molecule-graphene-nanoribbon junction
Vincent Pohl, Germany

PO2-255 Testing semiempirical quantum mechanical methods on model systems relevant to computer-aided drug design
Kristian Kříž, Czech Republic

Poster Session 2 – Tuesday, 29 August 2017

supported by The Journal of Physical Chemistry

PO2-256 Modulation of a weakly coupled peroxo-dicopper(II) complex by interaction with alkali metal ions
Lorenzo D'Amore, Spain

PO2-257 The case of endohedral boroshperene supersalt FLi2@B39 and its "super" properties
Anton Stasyuk, Spain

PO2-258 Simulating overtone induced chemistry with AIMD
Teemu Järvinen, Finland

PO2-259 New insights regarding chemical bonding within heavier analogues of ethers: siloxanes, germoxanes and stannoxanes
Ionut-Tudor Moraru, Romania

PO2-260 A DFT study on the reduction of CO2 to silylformates catalyzed by Ir-NSiN species
Victor Polo, Spain

PO2-261 High-level theoretical rovibrational spectroscopy of HCN
Benjamin Schröder, Germany

PO2-262 What are the physical contents of HDvV and Hubbard Hamiltonian parameters in the BS-DFT approach?
Grégoire David, France

PO2-263 Predictive multi-scale modelling: from atoms and electrons to drugs and airplanes
Judith Rommel, United Kingdom

PO2-264 Investigating complex formation of C99 with gamma-secretase, utilizing atomistic MM-MD simulations and free energy calculations
Manuel Hitzenberger, Germany

PO2-265 Quantum chemical calculation of electron ionization mass spectra for general organic and inorganic molecules
Christoph Bauer, Germany

PO2-266 Computational kinetics of industrially relevant carbonylation reactions from renewable resources
Emilija Kohls, Germany

PO2-267 Quantum-chemical investigations on photocatalytically active covalent organic frameworks
Gökcen Savasci, Germany

PO2-268 Quantized thermodynamic properties from the analysis of smoothed trajectories
Dénes Berta, Hungary

PO2-269 State-average analytical gradients and multireference perturbation theory for density matrix renormalization group (DMRG)
Leon Freitag, Switzerland

PO2-270 Enantioselectivity and computations: random phase approximation for a hydroboration reaction
Paola Nava, France

PO2-271 Direct dynamic DFT study of possible reaction mechanism of low-k SiOCH films with nitrogen atoms
Ekaterina Voronina, Russian Federation

PO2-272 Recent advances in interactive quantum chemistry
Adrian Mühlbach, Switzerland

PO2-273 Screening methods for linear-scaling short-range hybrid DFT calculations on CPU and GPU architectures
Matthias Beuerle, Germany

PO2-274 Multiscale modeling of interfaces in photovoltaic devices
Ulrik G. Vej-Hansen, Denmark

PO2-275 Chemistry and physics at semi-infinite surfaces using the surface Green's function method
Jess Wellendorff, Denmark

PO2-277 A genetic algorithm for the 3D structure prediction of peptides & proteins
Murat Kılıç, Switzerland

PO2-278 Radical N-heterocycle molecules: from excited states calculations to new molecular design
Arnaud Jaoul, France

PO2-279 Searching the growth mechanism of molybdenum disulfide: Atomic layer deposition under an electric field
Fabian Pieck, Germany

PO2-280 Spin-dependent effects in electronic devices
Martin Sebastian Zöllner, Germany

PO2-281 Explicitly dipole-polarizable, coarse-grained force fields from first principles
Frank Uhlig, Germany

PO2-282 Catalase actvity of manganese(III) complexes
Adrian Romero, Spain

PO2-283 An automated approach for structural characterization of complex organic compounds by collisional cross section computation
Sarah Moe, United States

PO2-284 Uncovering mechanistic details in organometallic catalysis - a combination of computation and experiment
Indrek Kalvet, Germany

Poster Session 2 – Tuesday, 29 August 2017

supported by The Journal of Physical Chemistry

PO2-285 Calculation of the excited state properties of molecular photocatalysts based on Ruthenium and Osmium
Miłosz Martynow, Poland

PO2-286 Core-level spectroscopy with the GW approximation
Dorothea Golze, Finland

PO2-287 Photophysical and photochemical properties of nitrobenzene from a static and dynamics perspective
Angelo Giussani, United Kingdom

PO2-288 Reparameterization of PM6 parameters for manganese and applications to binuclear manganese complexes
Toru Saito, Japan

PO2-289 Mechanism of oxidative enolate dimerizations elucidated through computational and experimental investigations
Emanuela Jahn, Czech Republic

PO2-290 Quantum mechanical scoring of protein-ligand binding enhanced with explicit-solvent effects
Cemal Köprülüoğlu, Czech Republic

PO2-291 A theoretical study on catalytic activity of h-BN monolayer by doping C atoms
Min Gao, Japan

PO2-292 Dynamics of chloroethylene resonant anions surveyed by bound state and scattering calculation
Fabris Kossoski, France

PO2-293 Conformational entropy of claisen rearrangement calculated by rate constant matrix contraction method
Yosuke Sumiya, Japan

PO2-294 A mechanistic investigation of the biomimetic ligand hydroxylation in Coppy-oxygen complexes
Jonas Peschina, Germany

PO2-295 Rotational tunneling of coupled methyl quantum rotors in γ-picoline crystal within a pair-coupled model
Somayeh Khazaei, Germany

PO2-296 The effect of substituents on the reactivity of keteniminium salts – a DFT study
Gamze Tanriver, Turkey

PO2-297 The generalized Bethe-Goldstone equation revisited: an incremental route towards the full configuration interaction limit
Janus Juul Eriksen, Germany

PO2-298 Envisioning CO2-HCHO conversion, C-H activation catalysts and anisotropy in actinide molecular nanomagnets: theoretical exploration
Tulika Gupta, Germany

PO2-299 General fit-basis functions and specialized coordinates in an adaptive density-guided approach to potential energy surfaces
Emil Lund Klinting, Denmark

PO2-300 The effect of ions on the clustering of organic acids and sulfuric acid
Nanna Myllys, Finland

PO2-301 Sulfoxide as a chirality information "storage device" to perform enantioselective arylation: how does it work?
Boris Maryasin, Austria

PO2-302 Efficient calculation of NMR shieldings including environmental effects
Kevin Reiter, Germany

PO2-303 Automated workflows for molecular simulation and force field calibration
Koen Visscher, Netherlands

PO2-304 Theoretical investigations of biomimetic iron(IV)-oxo complexes
Dieter Faltermeier, Germany

PO2-305 A sequential-QM/MM study of the electronic spectra of photochromic switches
Marcelo Hidalgo Cardenuto, Brazil

PO2-306 Accurate Intermolecular potential for the C60 dimer
Dmitry Sharapa, Germany

PO2-307 Theoretical investigation of the interaction of CO with Pd/MOR catalyst
Lenin Díaz, Brazil

PO2-308 Quantitative prediction of diastereoselective radical addition reactions
Mikko Muuronen, Germany

PO2-309 Fast Molecular Crystallization: Crystal Phase Transition Determines the Molecular Packing Kinetics
Cheng Shang, China

Poster Session 3 –Thursday, 31 August 2017

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Theoretical study of a lipase-catalyzed reaction in organic solvent
Eva Pluharova, Czech Republic

Temperature-dependent Triplet State Decay of Ir(ppz)2(F2ppy): role of metal centered state
Xu Zhang, China

Mechanism of drug resistance of chloroethylnitrosoureas mediated by O6-alkylguanine-DNA alkyltransferase: an ONIOM investigation
Lijiao Zhao, China

A wave function model for magnetic clusters
Tilmann Bodenstein, Denmark

The impact of cholesterol flip-flop and concentration on the plasma membrane
Sebastian Thallmair, Netherlands

Thermodynamic aspects of the electrocatalysis of proton reduction by diiron benzenedithiolate carbonyl complex
Mihajlo Etinski, Serbia

Accelerated dynamics simulations of supramolecular ruthenium-based water oxidation catalysis
Joachim Lindner, Germany

Spontaneous insertion and interaction of non-structure 3 protease protein domain with PIP2-containing membrane
Hung Minh Huynh, Belgium

Theoretical insights of supramolecular assembly on 2D atomic crystals
Hongde Yu, China

Structural properties and THz spectroscopic fingerprints of microsolvated ion-water clusters
Prashant Kumar Gupta, Germany

Density functional theory predictions of self-assembly on metal surfaces: is it successful?
James Hooper, Poland

Energetics of proton coupled-electron transfer reactions in the NADH-binding site of respiratory complex I
Patricia Saura, Germany

Rational design of single molecule magnets
Asha Roberts, Germany

Computational DFT-D3 and amber FF study of Z-DNA and its sugar-guanine stacking motif
Holger Kruse, Czech Republic

Linking protein motion and function: combining Markov state modelling and hybrid quantum mechanics/molecular mechanics
Eliot Boulanger, Belgium

From surfaces to nanoparticles: Ab-initio study of ruthenium oxide and its interaction with water
Javier Heras-Domingo, Spain

Unexpected contrast and "dark contours" in chiral STM markers
Ana Sanz Matias, Belgium

A quantum-chemical study of the DNA base-excision repair of 8-oxoguanine
Andrea Kreppel, Germany

Quantum entanglement within the polarization propagator approach
Leonardo Millán, Argentina

RmatReact: developing novel theoretical methodology to investigate ultra-cold atom-molecule collisions over deep potential wells
Laura McKemmish, United Kingdom

From sequence to function, QM/MM and virtual screening identify enzyme function and substrate scope
Marco Bocola, Germany

Probability current analysis and the charge transfer integral in organic semiconducting materials
Sang-Yeon Hwang, Republic of Korea

Pairwise specific reaction parameterization: a straightforward approach to improve semiempirical QM methods
Antoine Marion, Germany

Quantum-chemical calculations on the influence of molecular dipole moments on conformational equilibria
Johannes Dietschreit, Germany

Reduced scaling explicitly correlated coupled cluster methods for large molecular systems
Fabijan Pavosevic, United States

Efficient and accurate Born-Oppenheimer molecular dynamics for large molecular systems
Laurens D. M. Peters, Germany

Resonant inelastic X-ray scattering amplitudes and cross-sections in the ADC/ISR framework
Dirk Rehn, Sweden

Simulation of absorption and emission spectra of Laurdan in bilipid layer systems
Mirza Wasif Baig, Czech Republic

Reaching graphene-water systems: a new electronic-structure-based force field
Sergi Ruiz-Barragan, Germany

Site-occupation embedding theory using Bethe ansatz local density approximation
Bruno Senjean, France

Poster Session 3 –Thursday, 31 August 2017

supported by ACS Publications

Chemical dyanmics simulations to study tandem mass spectrometry peptide fragmentation: polyprolines series [pron-H]- as example
Ana Martin-Somer, Spain

Oxidation of metallocenes as external stimuli to enhance the reactivity of catalytically active metal complexes
Stephan Kohaut, Germany

Electronic structure and reactivity with alkenes of iron carbenes complexes: Towards iron-based olefin metathesis
Xavier Solans-Monfort, Spain

Enhanced sampling methods at the bio-inorganic interface: insights on silica biocompatibility and nanotoxicity
Massimo Delle Piane, Germany

Understanding the gas-phase fragmentation mechanisms of deprotonated L-cysteine-sulfate via direct dynamics simulations
Veronica Macaluso, France

Molecular dynamics applied to peptide nanotubes in a membrane environment
Martin Calvelo Souto, Spain

Assemblage of metal hydrides clusters: theoretical design of one and two-dimensional structures for hydrogen storage
Franklin Ferraro Gómez, Colombia

Alchemical free energy calculations by ensemble dynamics: The Conveyor Belt Scheme
David F. Hahn, Switzerland

Electron correlation from a screened Coulomb formalism
Daniel Kats, Germany

Bringing DORI to analyze and understand fluxional molecules
Benjamin Meyer, Switzerland

Combining molecular docking and QM/MM methods for studying ligand binding to metalloproteins
Okke Melse, Germany

Vibrational properties of iridium and rhenium complexes in ground and excited states: interpretation using DFT
Martin Pižl, Czech Republic

Molecular excitation energies from the Bethe-Salpeter equation
Xin Gui, Germany

Modelling the structural and optical properties of supramolecular arrays adsorbed on two-dimensional materials
Anton Nizovtsev, United Kingdom

Relativistic corrections for L=1 atomic states calculated with a finite-nuclear-mass approach and all-electron ECG functions
Monika Stanke, Poland

Excited states with second order approximate internally-contracted multireference coupled-cluster linear response theory
Arne Bargholz, Germany

Molecular dynamics simulation steady-state prediction by electrostatics — applications in supramolecular chemistry
Jean-Noël Grad, Germany

Using DFT methods to understand the chemistry of functionalized binary and intermetalloid Zintl clusters
Lukas Guggolz, Germany

Can coupled cluster theory describe polyradical character?
Andrew James, United States

Modeling sigma-Alkane complexes as pecursors to organometallic catalysis in solid-state
Tobias Kraemer, United Kingdom

Molecular basis of ligand interaction of GPR40/GPR120 based on FMO calculations with multiple sequence analysis
Yuta Yamamoto, Japan

Molecular dynamics simulation study of self-organization of carbazole dendrimer
Michio Katouda, Japan

Benchmark Ab Initio conformational energies for the proteinogenic amino acids and assessment of DFT functionals
Manoj Kumar Kesharvani, Israel

The model of multistage non-equilibrium electron transfer reaction in non-Debye polar solvent
Serguei Feskov, Russian Federation

Efficient parallel implementation of exact exchange for periodic systems within concentric atomic density fitting approximation
Xiao Wang, United States

A novel method for recruiting global optimization techniques for strategically oriented molecular simulation
Leila Lotfikatooli, Islamic Republic of Iran

Controlling the photoexcited decay of Fe(II)-N-heterocyclic carbene complexes through structural modifications
Matyas Papai, Denmark

Structure of hyaluronan solvation sphere and its influence on the molecular shape
Marek Ingr, Czech Republic

Carbon-chlorine multiple bonding in doubly and triply charged chlorobenzene
Felipe Fantuzzi, Brazil

Poster Session 3 –Thursday, 31 August 2017

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Towards improved machine learning and semiempirical quantum chemical methods
Pavlo Dral, Germany

CASPT2 on-the-fly surface hopping dynamics
Jae Woo Park, United States

Insights into the excited state chemistry of lanthanoid(III) motexafins
Norah Heinz, Germany

Orbital locality landscapes
Charles J C Scott, United Kingdom

Hybrid approach to fermi operator expansion: towards langevin dynamics with linear system-size scaling
Hendrik Wiebeler, Germany

Esterase-2 as a fluorescent biosensor for the detection of organophosphates: electronic insights from molecular dynamics
Ingrid Guarnetti Prandi, Brazil

CYLview: a free molecular analysis and representation program for chemists
Claude Legault, Canada

Range-separated hybrid scheme combining AP1roG with density-functional theory
Odile Franck, Poland

Electrode effects in molecular electronics: a computational perspective
Manuel Smeu, United States

The methylsulfinyl radical and its reaction with ozone
Marissa Estep, United States

Computational studies of substituted porphyrin-squaraine dyads as chromophores for solar cells based on TiO2
Merlys Borges-Martinez, Chile

Laplace-transformed atomic and active orbital-based formulations of relativistic and multireference perturbation theories for large molecules
Benjamin Helmich-Paris, Netherlands

Calculating lower bound to the energy eigenvalues of the Hamiltonean
Zsuzsanna Tóth, Hungary

Holomorphic Hartree-Fock theory: beyond the Coulson-Fischer point
Hugh Burton, United Kingdom

The prototypical transition metal carbenes: (CO)5Cr=CH2, (CO)4Fe=CH2, and (CO)3Ni=CH2
Jared Weidman, United States

Contributions for the combustion model of dimethyl ether from theoretical calculations
Glauco Bauerfeldt, Brazil

Multistructure and multipath kinetics test study: reaction of 1-pentene + OH
Tatiane Tejero, Brazil

Computational study of isolated glycine, alanine and solvated glycine zwitterion and contribution to ISM behavior
Neubi Xavier, Brazil

Keteniminium salt formation and their electrocyclization reactions
Ulfet Karadeniz, Turkey

Fermionic PEPS for finite two-dimensional Hubbard models
Jheng-Wei Li, United States

Electron delocalization in infinite σbonded one-dimensional chains (MMe2)∞, M = Si, Ge, Sn, Pb
Milena Jovanovic, United States

Structural characterization of hydrogen adsorbed ruthenium clusters - toward an atomistic understanding of ammonia synthesis
Anna-Sophia Hehn, Germany

DFT study of the chemical-physics properties of a series of new benzoxazole derivatives
Dalila Hammoutène, Algeria

Development of In Silico drug design techniques based on the fragment molecular orbital method
Kaori Fukuzawa, Japan

Construction of IFIE-database with semi-automated FMO calculation protocol
Chiduru Watanabe, Japan

New insights into oxygen activation on nanoporous gold: a selective catalyst for methanol oxidation
Wilke Dononelli, Germany

Mechanism of Nakamura's bisphosphine iron-catalyzed asymmetric C(sp2)-C(sp3) cross-coupling reaction
Osvaldo Gutierrez, United States

Theoretical study on the origin of the enantioselectivity of flexible catalytic systems
Miho Hatanaka, Japan

Proton transfer in cytochrome c oxidase - calculation and prediction of transition networks
Marco Reidelbach, Germany

The effects of Lewis acid complexation on type I radical photoinitiators
Benjamin Noble, Australia

Poster Session 3 –Thursday, 31 August 2017

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Advanced artificial neural network approaches to prediction of pharmacokinetic properties and toxicity of drug com pounds
Eugene Radchenko, Russian Federation

How many electrons are excited in an electronic transition?
Giuseppe Barca, Australia

Photoisomerisation and electronic spectroscopy of XC3N (X=-CH3, -H). The TD-DFT perspective
Marcin Gronowski, Poland

Boron-doped graphene for multifunctional coating - A DFT study
Valentina Cantatore, Sweden

Theoretical design of boron nitride based electrocatalysts for oxygen reduction and hydrogen evolution reactions
Andrey Lyalin, Japan

Analysis of hyperfine structure in Dirac theory: anomalous increase of relativistic contraction of outer orbitals
Ayaki Sunaga, Japan

An open-source framework for analyzing N-electron dynamics. capabilities and applications of detCI@ORBKIT
Gunter Hermann, Germany

Structural and spectroscopic investigation of acetyl cyanide: theory and experience
Ayad Bellili, France

Exciton relaxation dynamics in photoexcited cycloparaphenylenes
Ljiljana Stojanovic, France

Water adsorption on gold nanoparticles: a theoretical approach
Chen Hui Chan, France

Knockout driven reactions in porphyrin molecules and butadiene clusters
Giovanna D'Angelo, Spain

QM/MM studies of reactive intermediates in solution: diphenylcarbene in solvent mixtures
Pandian Sokkar, Germany

Time-dependent extension of the long-range corrected density functional based tight-binding method
Julian J. Kranz, Germany

Mechanism of the photochemical ligand substitution of fac-[ReI(bpy)(CO)3(PR3)]+ complex
Kenichiro Saita, Japan

Vibrational density matrix renormalization group
Alberto Baiardi, Italy

Molecular response to strong magnetic fields: excitation energies and anapole moments
Sangita Sen, Norway

QM/MM polarizable embedded RI-CC2 analytical gradients: deexcitation pathways of a triazene compound in complex environments
Alireza Marefat Khah, Germany

On-the-fly ab initio semiclassical dynamics of floppy molecules: resonance Raman spectra of ammonia
Sebastien Reynaud, Switzerland

Correlation between the activity of lipase and differences in binding free energies
Sindrila Dutta Banik, Denmark

The independent gradient model: a tool derived from the NCI approach to analyze molecular interactions
Eric Henon, France

Replica-exchange enveloping distribution sampling (RE-EDS): parallel energy-offset estimation and efficient local round-trip time optimisation
Dominik Sidler, Switzerland

Carbon monoxide activation on Ru surfaces under reaction conditions from Ab initio molecular dynamics simulations
Lucas Foppa, Switzerland

Refined approach to the cellularization of the semiclassical Herman-Kluk propagator
Sergey Antipov, Switzerland

Local control theory with an approximate treatment of the molecule-field interaction
Julien Roulet, Switzerland

Probing the orientation of recombinant protein A on a membrane using computational infrared spectroscopy
Ana Cunha, Netherlands

Color-tuning mechanism in vision from a theoretical perspective
Boris Kamorzin, Russian Federation

Accurate prediction of protein-ligand binding using molecular dynamics-based docking and QM/MM methods
Iris Antes, Germany

Symmetric proton transfer routes in the membrane domain of respiratory complex I
Andrea Di Luca, Germany

Aggregates of quadrupolar Dyes: the Role of Intermolecular Interactions
Olatz Uranga, Spain

Theoretical study of the BrO + ClO cross reaction
Adam Abbott, United States

Poster Session 3 –Thursday, 31 August 2017

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Structural distortions accompanying non-covalent interactions
Herzain Isaac Rivera-Arrieta, Mexico

Solubility of diclofenac in water: interplay between intra- and intermolecular hydrogen bonds
Mariana Kozlowska, Poland

Can orbital-based decomposition of nonlinear optical properties unveil the role of electron correlation?
Sebastian Sitkiewicz, Spain

Excited state gradients for a state-specific continuum solvation approach: a lagrangian TDDFT formulation of VEM
Ciro Achille Guido, France

Coherent dynamics in photoexcited azobenzene: ultrafast decay resolved by sub-20-fs pump-probe spectroscopy and theoretical simulations
Artur Nenov, Italy

Atmospheric photoisomerization interference in the gas-phase oxidation of E,E-2-4-hexadienal with OH: the Ketene-aldehyde equilibria
Rene Pfeifer, Brazil

Dissipative particle dynamics study of poly(N-isopropylamide) with carboxylic and dodecyl terminal groups in aqueous solutions
Karel Šindelka, Czech Republic

Template-catalysed formation of cyclohexanohemicucurbiturils
Toomas Tamm, Estonia

Variational transition state theory study of radical reactions
Xuefei Xu, China

Different QM/MM approaches to study enzymatic reactions: ppGalNAcT2 glycosyltransferase
Pavel Janoš, Czech Republic

On-the-fly ab initio semiclassical evaluation of absorption spectra of polyatomic molecules beyond the Condon approximation
Tomislav Begusic, Switzerland

AlgoGen: a program to perform molecular docking with full quantum refinement (DFQR)
Hassan Khartabil, France

Efficient Eigensolvers for linear response time-dependent density functional theory
Jiri Brabec, Czech Republic

Compressed representations of dispersion interactions and long-range electronic correlation
Jerome F. Gonthier, United States

State-of-the-art solvation free energy modelling - add more physics and do without fudge factors
Lars Sandberg, Sweden

Thermodynamic modelling of mesophase pitch for the development of high-performance carbon fibers
Caio Florindo, Brazil

Hydrogenation of phenyl substituted unsaturated functional groups by d5 and d6 metal substituted PNP complexes
Zhihong Wei, Germany

Adsorption and activation of water on cuboctahedral Rh and Pt nanoparticles
Andrey Bazhenov, Finland

Symmetric dissociation and excited states with selected configuration interaction with truncation energy error
César Xavier Almora Díaz, Mexico

An interpolation approach for the choice of polarization functions when using Gaussian basis sets
Ana Mora, Brazil

Theoretical pKa calculations of difficult cases for thermodynamic cycles: amino acids and peptides
Rodrigo Casasnovas, Spain

Automatic differentiation in quantum chemistry: application in fully variational Hartree-Fock
Teresa Tamayo, United States

Why does MP2 outperform MP3 and how can we improve perturbation theory?
Reinhold Fink, Germany

Binary mixtures of ionic liquids with a common anion: a molecular dynamics study
André Melo, Portugal

Nonlinear optical properties from TDDFT: trials and tribulations
Shane Parker, United States

Challenges and procedures towards automated flow chemistry
Loïc Roch, United States

Relativistic effects on NMR spectroscopic parameters of atoms belonging to hydrogen-bonds
Teresita Santa Cruz, Argentina

Mechanisms of surface O removal by H2 and CO activation on Fe and Co surfaces
Haijun Jiao, Germany

The quantum biology of vitamin D - Insights from non-adiabatic dynamics
Enrico Tapavicza, United States

Poster Session 3 –Thursday, 31 August 2017

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Dual structure-based approach towards the design of inhibitors of the Dengue virus envelope protein
María Gabriela Aucar, Argentina

Benchmark noncovalent interaction energies: balancing databases and improving dispersion damping functions
Konrad Patkowski, United States

Explaining the NMR spectrum of the active site of photoactive yellow protein
Phillip Taenzler, Germany

Charge transfer of a prokaryotic (6-4) photolyase PhrB
Daniel Holub, Germany

Quantum vibrational spectroscopy of biomolecules using ab initio classical separable potentials
Barak Hirshberg, Israel

Studying the nature of hydride transfer and its role in the enzymatic catalysis
Rafael Garcia Meseguer, Spain

Insights into the photochromism of a red/green cyanobacteriochrome
Christian Wiebeler, Israel

Global optimization, analysis and simulation - the recent developments within the CAST program
Dustin Kaiser, Germany

Dispersion-corrected DFT study of enantiospecific adsorption of amino acids on hydroxylated quartz surfaces
Alastair Price, Canada

Minimum energy path calculations accelerated with Gaussian process regression
Vilhjálmur Ásgeirsson, Iceland

Theoretical investigation into the enzymatic excision mechanism in AP endonuclease (Ape1)
Hossein Batebi, Germany

Steering orbital optimization out of local minima and saddle points toward lower energy
Alain Vaucher, Switzerland

Soft matter morphologies with atomistic resolution from Coarse-Grain solvent evaporation simulations
Riccardo Alessandri, Netherlands

Highly accurate dipole transition probabilities in molecules from finite-field relativistic multireference coupled cluster calculations
Ephraim Eliav, Israel

Trying to unravel the mechanisms of cytotoxicity for the [Mo(η3-C3H5)Br(CO)2(phen)] complex: Intercalation vs. Groove Binding
Adrià Gil-Mestres, Portugal

DFT study of heterobimetallic complexes derived from the e-deficient Ru-H complex, [Ru(IPr)2(CO)H]+
Nasir A Rajabi, United Kingdom

Central fields from Jensen´s form
Jan Linderberg, Denmark

A theoretical study of CO dissociation and C-C bond formation mechanism on Fe(710)
Teng Li, Germany

Structural assignment, electronic and magnetic properties of $Si_7M_0^{-}$ with M = Pr, Gd, Ho
Dieu Hang Tran, Belgium

Modelling photoinduced events and non-linear spectroscopy in complex multichromophoric systems
Francesco Segatta, Italy

Localization errors and controllable sparsity in the coupled-cluster wave function for time-dependent response theory
Rachel Glenn, United States

Investigating ϖ-acid-base interactions of supramolecular cyclic trinuclear coinage metal complexes
Fabian Bohle, Germany

Explicitly correlated electronic structure methods: progress towards increasing efficiency
Travis Hunter Thompson, Germany

Understanding chemical bonding in terms of electronic correlations
Gergely Barcza, Hungary

Proton coupled electron transfer and competing mechanisms in free radical reactions in aqueous solutions
Ivana NikšićFranjićCroatia

Modelling PtII(Ligand) - amyloid-βinteractions: prediction of ligand effects
Matthew Turner, United Kingdom

Double residues of response functions in density matrix-based response theory
Daniel H. Friese, Germany

Hydrogenation of carbon dioxide over magnesium and copper alkoxide-functionalized metal-organic framework
Daniela Guzmán-Angel, Chile

Efficient implementation of the approximate exchange kernel method
Guo Chen, United States

Many-fermion tunneling through a barrier
Elke Fasshauer, Denmark

Poster Session 3 –Thursday, 31 August 2017

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Quantitative analysis of axial chirality in biaryl and related compounds
Inbal Tuvi-Arad, Israel

Understanding the crystallization tendency of sulfadiazine and sulfamerazine in different solvents
Geoffrey Wood, United States

Generalized coupled-cluster approaches for quantum simulation of strongly correlated system
Jhonathan Romero, United States

A consistent molecular model to predict the behavior of early tetravalent actinides
Eleonor Acher, France

The PNO-MP2 gradient and its application to molecular geometry optimizations
Marius Frank, Germany

Magnetically induced currents in organic boron-nitrogen polycyclic molecules and organic ring systems containing metal ions
Maria Dimitrova, Finland

Valence bonds in elongated boron clusters
Athanasios Arvanitidis, Belgium

Complexation of some divalent cations with morin: a spectroscopic and theoretical study
Aurélien Moncomble, France

Li2H vibrational energy levels from a new global ab initio potential energy surface
Denis Hagebaum-Reignier, France

The catalytic mechanism of GatA: a molecular dynamics and QM/MM study
Paul Meister, Canada

The 340-cavity in neuraminidase provides new opportunities for influenza drug development
Nanyu Han, China

A reliability parameter for frozen-density embedding calculations
Alexander Zech, Switzerland

Computer modelling of FRET-based protein nanosensors
Joshua Mitchell, Australia

Tensor-decomposed vibrational coupled-cluster theory
Niels Kristian Madsen, Denmark

Inhibition mechanisms of cathepsin B: a theoretical study
Anna Heilos, Germany

Methane activation by titanium neopentylidene complexes: modification of the ligands
Dragan Ninkovic, Qatar

Computational investigations for Cu-catalyzed site-selective arylation of indoles: the directing group effects
Ting Wang, China

Interplay of orbital breathing and electron correlation in corner-sharing cuprates
NIkolay Bogdanov, Germany

Mono- and di- alkylation processes of DNA-bases by anticancer drug mechlorethamine
Olatz Larrañaga, Spain

The interaction of complex biomolecules with zeolitic layers: ab initio and molecular dynamics study
Miroslav Rubes, Czech Republic

Analytic open-shell local MP2 gradients using intrinsic bond orbitals
Mark Dornbach, Germany

The zwitterionic nature of tetrasilatetramide Si4{N(SiMe3)Dipp}4 - quantum chemical characterization of a small silicon cluster
Christian Mück-Lichtenfeld, Germany

Empirical charge scheme for transition metals and lanthanoids: development and applications
Bodo Martin, Germany

Explicit-implicit embedding strategy to calculate Raman and Raman optical activity spectra of solvated systems
Tommaso Giovannini, Italy

An accurate force field for both folded and disordered states of peptides and proteins
Hao-Nan Wu, China

Rotational constants and vibrational spectra of acenaphthene water complexes
Jens Antony, Germany

A scalable and efficient approach to polarizable force fields in molecular dynamics simulations
Jonathan Coles, Germany

Properties of molecular magnets
Andreas Nyvang, Denmark

Solvent dynamics controls the Schlenk equilibrium of Grignard reagents: computational study of CH_3MgCl in tetrahydrofuran
Raphael Peltzer, Norway

A rational look at fluorescent proteins through excited state reaction path calculations

Poster Session 3 –Thursday, 31 August 2017

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Daryna Smyrnova, Belgium

Controlling electron transfer through selective vibrational excitation
Theo Keane, United Kingdom

Improving AMBER non-bond parameters for inorganic and alkyl oxoanions, when experimental data is not available
Sadra Kashef Ol Gheta, Germany

Computationally guided design of transition metal PXP pincer complexes for NH3 fixation
Julen Munarriz, Spain

How reliable is density functional theory to describe uranium-based molecular compounds?
Daniel Reta, United Kingdom

Prediction of DFT-derived point-charges using a machine learning model
Patrick Bleiziffer, Switzerland

Description and modelling of spectra, structure and function of Histidin Kinase Rhodopsin (HKR)
Franziska Beyle, Germany

Characterization of the intermediate states of transport cycle of sodium symporters via transition-path sampling methods
Ina Bisha, Germany

Implications of axial coordination on the Redox behavior and H-atom-abstraction reactivity of compound I analogues
Mauricio Maldonado-Dominguez, Czech Republic

Shedding UV-light on the origins of RNA nucleotides
Rafał Szabla, Poland

Domain-based local pair natural variant of Mukherjee´s multireference coupled cluster method
Ondrej Demel, Czech Republic

Modeling and NMR calculations of oximes in water and ionic liquids: solvation shell structure implications
Alexandre Alves de Castro, Brazil

Mechanistic insights into the selective hydrolysis of Asp-X peptide bonds in proteins by Zr(IV)-substituted polyoxometalates
Tzvetan Mihaylov, Belgium

Excitons and charge transfer states in light-harvesting antenna complexes
Lorenzo Cupellini, Italy

O(n) concentric atomic density fitting for Hartree-Fock exchange
Cannada Lewis, United States

The intricate case of tetramethyleneethane
Libor Veis, Czech Republic

DFT investigation on the trans-cis C-Pd-C rearrangement in heteroleptic Pd-hemichelates
Sebastian Dohm, Germany

Coarse grained cross-scale expression of complex combustion reaction mechanism based on master equation
Lin Ji, China

Soft X-ray spectroscopy of transition metal compounds: a theoretical perspective
Sergey Bokarev, Germany

Elucidating the structure of merocyanine dyes with the ASEC-FEG method
Herbert Georg, Brazil

Accelerating equilibrium isotope effect calculations by stochastic change of mass
Konstantin Karandashev, Switzerland

Describing chemical reactions in explicit solvent using adaptive QM/MM models
Jelle Boereboom, Netherlands

Time-resolved X-ray scattering by non-stationary states in atoms and molecules
Mats Simmermacher, Denmark

Towards highly accurate correlation energies for molecular systems
Jian-Hao Li, Switzerland

Mechanistic investigation of solvent-controlled CO_2 reduction by triphos-iron-hydride complex
Abhishek Khedkar, Germany

Detailed mechanistic studies on palladium/norbornene catalyzed C-H amination of aryl halide
Ping Chen, China

Enhancing fluctuations in chemical reactions
GiovanniMaria Piccini, Switzerland

Ultrafast spin-flip dynamics in transition metal complexes triggered by soft X-ray light
Oliver Kühn, Germany

Theoretical investigations of sigma-hole interaction in condensed halogen systems
Carsten Müller, Germany

Theory of strong-field effects in femtosecond electronic two-dimensional spectroscopy
Elisa Palacino-González, Germany

Virtual screening through molecular fingerprinting of existing antipsychotic drugs
Ashish Radadiya, United Kingdom

Poster Session 3 –Thursday, 31 August 2017

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Tunnex: a user-friendly program to compute tunneling kinetics
Henrik Quanz, Germany

Activation of the GTP hydrolysis by the Switch I region in the elongation factor EF-Tu
Bülent Balta, Turkey

Q-Chem 5: facilitating worldwide scientific breakthroughs
Evgeny Epifanovsky, United States

Finite temperature dynamics of a Holstein polaron: Thermo Field dynamics approach
Lipeng Chen, Germany

Applicability of the effective oxidation state analysis
Verònica Postils Ribó, Spain

Spectroscopy of cooperative laser electron-gamma-nuclear processes in molecules and clusters: new effects in cryogenic molecules
Alexander Glushkov, Ukraine

A detailed view into structural and functional mechanism of the first intermediate state of channelrhodopsin-2
Beatrix Bold, Germany

Spectroscopy interatomic potentials, collisional line shift and broadening for molecular pairs "heavy atom-noble gas atom"
Olga Khetselius, Ukraine

Exploring the structure of dialkyl and diallyl magnesium clusters by means of global search algorithm
Samira Bouaouli, France

New electron-beta-nuclear spectroscopy of molecules and chemical bond effect on the beta-decay parameters
Vasily Buyadzhi, Ukraine

A theoretical study of the interaction of calcite with amino acids
Robert Stepic, Germany

Solid-state and molecular size depending on variation of fundamental constants
Lukas F. Pasteka, New Zealand

Relativistic quantum chemistry of heavy elements and hadronic atoms and molecules
Valentin Ternovsky, Ukraine

Consistent approach to Raman scattering of the light on metastable levels of diatomic molecules
Eugeny Ternovsky, Ukraine

Theoretical photoelectron spectroscopy: a versatile tool to understand the electronic structure
Gilbert Grell, Germany

Theoretical determination of the ground state of CsS and CsO
Sihem Azizi, Algeria

Algorithm for calculating Bethe logarithm for two- or three- centered molecules
Ewa Palikot, Poland

Studys of anorganic biradicals: dependancy of computational methods, electronical and sterical effects
Eileen Welz, Germany

Competition between photolysis and spin-crossover : quantum wavepacket dynamics on heme-CO organometallic complex
Miquel Huix-Rotllant, France

Multilevel coupled cluster theory with Cholesky- and correlated natural transition orbitals for core-excited states
Sarai Dery Folkestad, Norway

Interrogating the "B05" density functional for non-locality information
Stephen Dale, Canada

High-accuracy extrapolated ab initio thermochemistry of the cyanonitrene radical
Michael Harding, Germany

Can wavefuntion analysis support the (new) definition of oxidation state?
Pedro Salvador, Spain

Excited states for orbital-optimized second-order perturbation theory
Eloy Ramos-Cordoba, United States

Energetic parameters of the Pt(SCN)62- complex
Vladislav Yudanov, Russian Federation

Theoretical study of the methanamine formation as glycine precursor in the ISM: role of water-ice
Francisca Alexandra Cid Mora, Chile

Squaramide polymerization of lactide: crucial role of a weak interactions network
Christophe Gourlaouen, France

Excited state transition energies and properties in solution from a smooth dielectric model
J. Coleman Howard, United States

On the chirality of antimalarial drug candidates
Kirk C. Pearce, United States

Electrochemistry via liquid photoemission spectroscopy: insight from molecular simulations

Poster Session 3 –Thursday, 31 August 2017

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Veronika Jurásková, Czech Republic

Numerically converged hyperfine coupling constants using a similarity transformed Hamiltonian and a multiwavelet basis set
Stig Rune Jensen, Norway

Interactions of binary twinned-icosahedral [B21H18]– with cyclodextrins
Saltuk Mustafa Eyrilmez, Czech Republic

Understanding and utilizing the role of London dispersion interactions in catalysis
Lijuan Song, Germany

Molecular Dynamics Simulations on the Aggregation of Keggin-Type Polyoxometalate Ions in Aqueous Solution
Alain Chaumont, France

Spin-orbit coupling matrix elements from the Hermitian formulation of coupled cluster response theory
A Tucholska, Poland

Upgrading existing GGA functionals to range-separated hybrid meta-GGAs
Marcin Modrzejewski, Poland

High-energy photochemistry in liquid solutions: Ultrafast proton and electron transfer initiated by X-rays
Daniel Hollas, Czech Republic

Lewis acid bulkiness effect on the stereoselectivity of cycloaddition reactions between acyclic dienes and α,β–enals
Diana Yepes, Chile

NMR magnetic shielding in halogen bonding and cooperative effects in (BrF)n clusters
Sandra Patricia Blatter, Argentina

Reaction Force Constant Analysis Applied in Organic and Organometallics Multi-Bond Reactions
Pablo Jaque, Chile

DLPNO-CCSD(T) based compound methods for accurate thermochemistry
Dimitrios G Liakos, Germany

Insights into heterogeneous catalysts from theoretical spectroscopy and accurate binding energies
Dimitrios Maganas, Germany

Energy decomposition analysis for studying covalent bonds
Daniel S. Levine, United States

Exact single-electron approach to the dynamics of molecules in strong laser fields
Axel Schild, Switzerland

When magnetism meets reactivity: hydrogen generation via a bi-metallic mechanism with spin exchange
Nuno A. G. Bandeira, Portugal

$FeNO_2$+ as a model system for spin-state energetics
Constantine Sakellaris, Germany

Orbital relaxation and electronic transitions - what is the nature of Handy´s Z-vector?
Thibaud Etienne, France

Stochastic-CASSCF and multiconfiguration pair-density functional theory for spin challenges in organometallic and organic chemistry
Giovanni Li Manni, Germany

Putting the squeeze on: First-principles melting of Hg, Cd and Zn under pressure
Krista G. Steenbergen, New Zealand

Oxygen induced diffusion of Ni atoms in Ni-Au clusters
Ralf Meyer, Austria

Adsorption of post-combustion gases by Mg-MOF-74
Xvaier Giménez, Spain

LiEBe2+ - ligand exchange at beryllium dications
Ralph Puchta, Germany

Hydride-enhanced ligand nucleophilicity for metalloorganic catalytic reactivities
Theo P. Goncalves, Saudia Arabia

Influence of odd/even alkyl side-chain substitution on the morphology and charge-transport of benzothieno-benzothiophenes (BTBT)
Ilhan Yavuz, Turkey

Calculation of Molecular Properties from Relativistic Electron Dynamics
Lukas Konecny, Slovakia

Dynamics of Photo-fragmentation of Methanol
Kritsana Sagarik, Thailand

Investigating the molecular structure and hydrogen bonding in single-chain polymer nanoparticle self-assembly binding motifs
Peter A. Limacher, Germany

Recent developments in domain local pair natural orbital electron correlation approaches.
Christoph Riplinger, Germany

Res-FEP: A tool for in silico site-directed mutagenesis in ligand-binding

Poster Session 3 –Thursday, 31 August 2017

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Hugo Gutierrez de Teran, Sweden

Virtual-reality view on chemistry and materials science
Ruben Jesus Garcia-Hernandez, Germany

Selective Transformation of Cyclic Vinyl Carbonates to Allylic Amines and Aldehydes - A DFT Study
Rositha Kuniyil, Spain

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General Information

Congress Venue

Gasteig Cultural Center
Rosenheimer Str. 5
81667 Munich
Germany

Opening hours of the registration desk

Sunday, 27 August 2017	12:00 - 19:30
Monday, 28 August 2017	08:00 - 19:00
Tuesday, 29 August 2017	08:30 - 19:00
Wednesday, 30 August 2017	08:30 - 14:00
Thursday, 31 August 2017	08:30 - 19:00
Friday, 1 September 2017	08:30 - 13:30

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During the congress, please wear your name badge at all times. The badge is your entrance ticket to the session halls.

Lectures

The length of the talks is as follows:

Plenary Lectures:	35 min talk + 5 min discussion
Invited Lectures:	20 min talk + 5 min discussion
Contributed Lectures:	12 min talk + 3 min discussion
Lectures in Industry Sessions:	20 min talk + 5 min discussion

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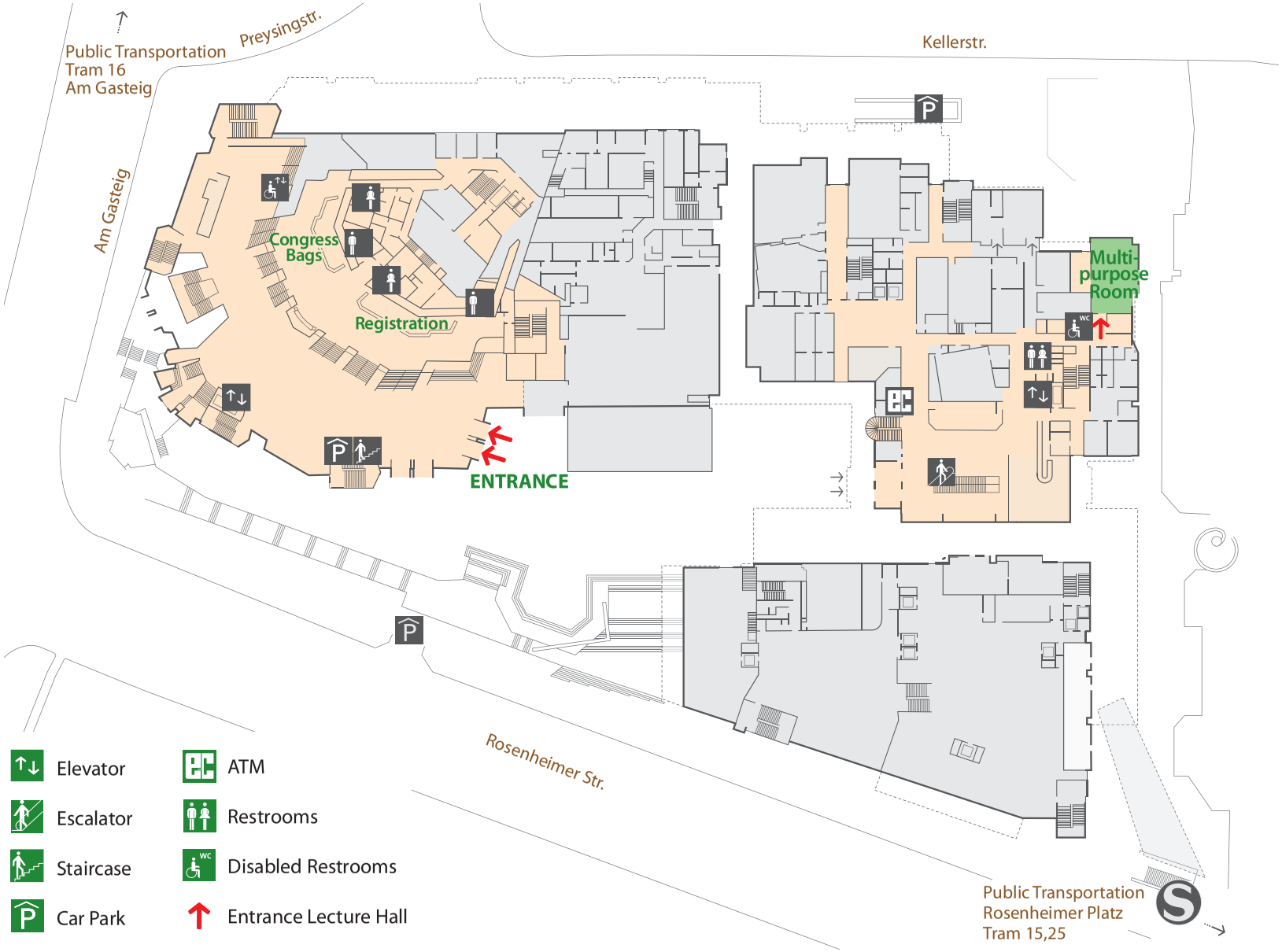
ACS Publications will kindly sponsor three poster awards for every poster session. The winners will be announced during the closing ceremony on Friday, 1 September. Attention: The winners of the poster awards need to attend the closing ceremony. If a winner is absent at the ceremony, the award will be awarded to the next candidate on the list.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Elevator
Escalator
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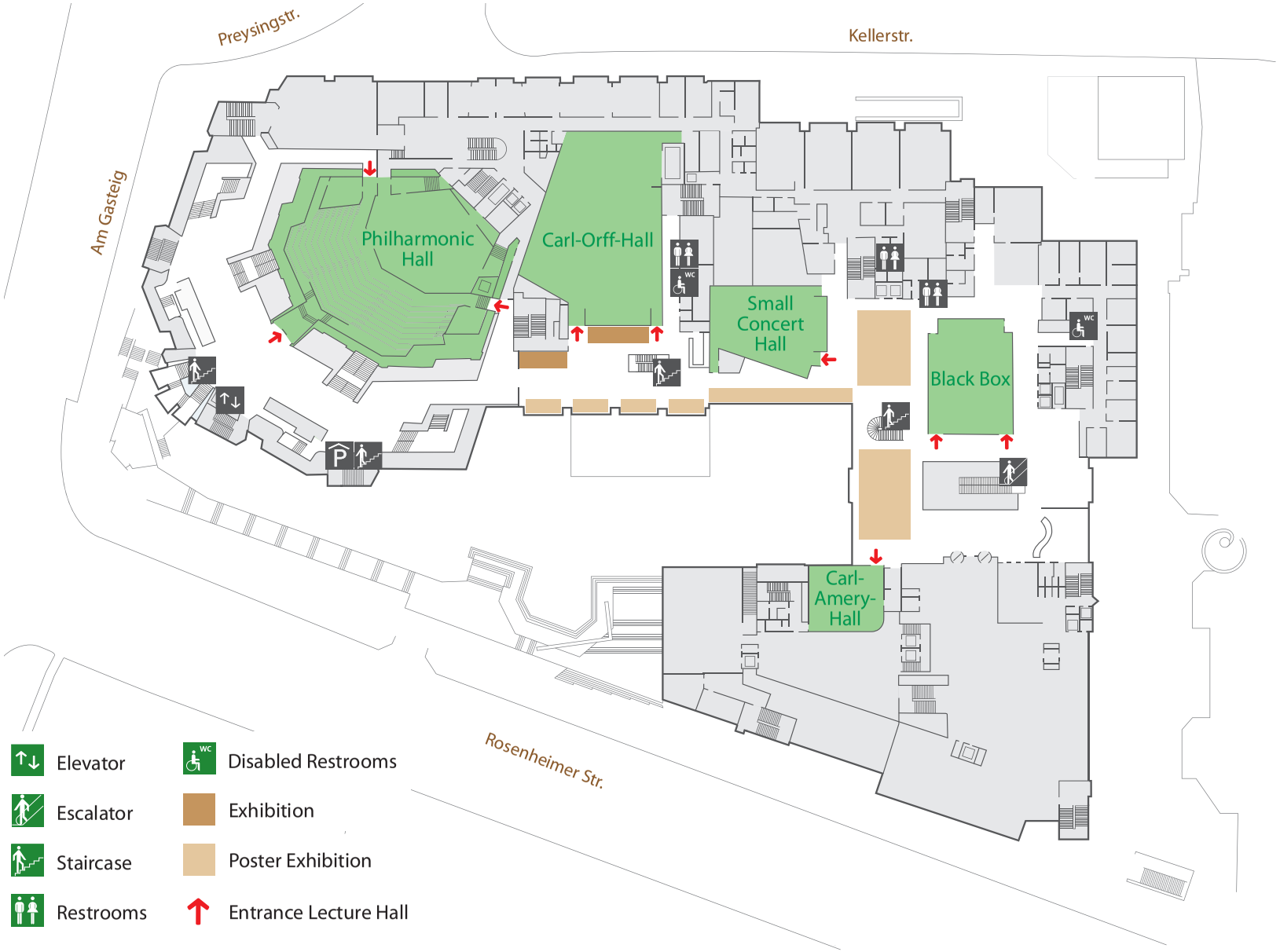
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Black Box
Carl-Amery-Hall
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Staircase
Restrooms
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Poster Exhibition
Entrance Lecture Hall

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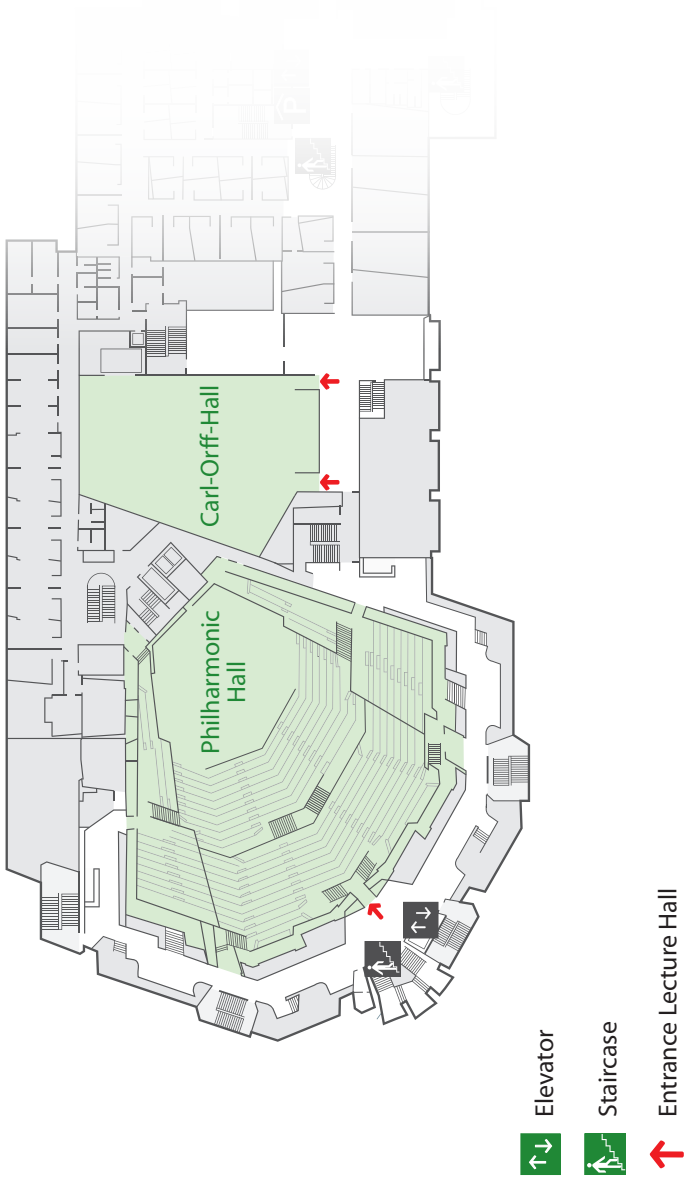

AUTHOR INDEX

Author Index

Author Index

Author Index

C

Author Index

D

Author Index

E

Author Index

F

Author Index

G

Author Index

H

Author Index

I

J

Author Index

K

Author Index

L

Author Index

M

Author Index

Author Index

N

O

Author Index

P

Author Index

Q

R

Author Index

S

Author Index

Author Index

T

Author Index

U

V

Author Index

Author Index

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