



WATOC 2017

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

27 August – 1 September 2017
Munich, Germany



SCIENTIFIC PROGRAM



LUDWIG-
MAXIMILIANS-
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MÜNCHEN

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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

List of Sponsors and Exhibitors

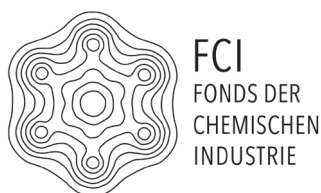
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Sponsors & Exhibitors





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 Neepe 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 Čárský	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 Björnsson Alister Page Olaf Wiest Dmitry Nerukh Laurence Leherste Xabier Lopez	Contributed Session 3 Shirin Faraji Oliver Kühn Debashree Ghosh Daniel Roca-Sanjuán Bo Durbec 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 Rezáč Ekaterina Pas	Contributed Session 8 Andrey Rogachev Carsten Baldauf Brian Yates Hélène Bolvin Masato Kobayashi Lubomír Rulišek 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 <i>The Journal of Physical Chemistry</i>					

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 Coitino 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 Lubner 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 Silvia Simon Ulrike Salzner Hong-Xing Zhang Martial Boggio-Pasqua Aurélien Perrier David Henry Thibaud Étienne	Contributed Session 17 José Enrique Barquera-Lozada Fabio Pichierri Andrés Stirling Leonardo Belpassi Apostolos Kalemios 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	
	OPENING CEREMONY <i>Chair: Christian Ochsenfeld</i>	
15:00 – 15:50	Opening Schedule: <i>Christian Ochsenfeld</i> (Chair of WATOC2017) <i>Walter Thiel</i> (WATOC President) <i>Barbara Conradt</i> (Vice President of the University of Munich (LMU)) <i>Helmut Schwarz</i> (President of Humboldt Foundation (AvH)) Music Intermezzo by <i>Ville Kaila</i> (violin), <i>Lika Bibileishvili</i> (piano)	
15:50 – 17:10	Plenary Session A <i>Chair: Peter Gill</i>	
15:50 – 16:30	PL-1	<i>Todd Martinez</i> Ground and excited state dynamics on graphical processing units
16:30 – 17:10	PL-2	<i>Benedetta Mennucci</i> 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 <i>Chair: Leo Radom</i>	
17:40 – 18:20	PL-3	<i>Trygve Helgaker</i> Quantum chemistry in magnetic fields
18:20 – 19:00	PL-4	<i>Helmut Schwarz</i> 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 <i>Chair: Kenneth Ruud</i> 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 <i>Chair: Thomas Jagau</i>		Invited Session 2 <i>Chair: Tim Clark</i>		Invited Session 3 <i>Chair: Tomasz Wesolowski</i>		Invited Session 4 <i>Chair: Hans Jørgen Aagaard Jensen</i>		Invited Session 5 <i>Chair: Manabu Sugimoto</i>		Invited Session 6 <i>Chair: Henry Rzepa</i>	
10:10	I-011	<i>Peter Gill</i> 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	<i>Hiromi Nakai</i> Chemical reaction simulations on CO ₂ chemical absorption process	I-061	<i>Odile Eisenstein</i> Can carbon-13 NMR chemical shifts inform on reactivity in organometallic chemistry?
10:35	I-012	<i>Garnet Chan</i> Notes on the complexity of electronic structure theory	I-022	Kwang Soo Kim Graphene nanoribbon based electronics and spintronics	I-032	Neepta Maitra Confronting memory-dependence in time-dependent density functional theory	I-042	<i>Pekka Pyykkö</i> Recent results on compounds of heavy, and heaviest elements	I-052	<i>Nuria Lopez</i> New aspects in the simulations of heterogeneous catalysis	I-062	<i>Michael Buehl</i> Exploring NMR properties of paramagnetic Cu phenolic oxime complexes
11:00	I-013	<i>Jürgen Gauss</i> 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	<i>Wenjian Liu</i> New Scenarios for Strongly Correlated Electrons	I-053	<i>Tore Brinck</i> σ -hole Bonding in the Catalysis of Nanostructured Metals: Surface Properties as Guides to Local Reactivity	I-063	<i>Gustavo Aucar</i> NMR spectroscopic parameters of HB containing molecules and aggregates of DNA base pairs
11:25	I-014	<i>Poul Jørgensen</i> 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	<i>Trond Saue</i> Variational perturbation theory in geochemistry	I-054	<i>Stuart Macgregor</i> Modelling alkane σ -Complexes in the solid state	I-064	<i>Ibon Alkorta</i> Anion-anion and cation-cation halogen and hydrogen bonded complexes
11:50	I-015	<i>Martin Head-Gordon</i> 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	<i>Marcel Swart</i> Characterization of reactive high-valent transition-metal complexes	I-055	<i>Michelle Coote</i> Directionality and the role of polarization in electrostatic catalysis	I-065	<i>Sotiris Xantheas</i> 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 <i>Chair: Henrik Zipse</i>		Invited Session 8 <i>Chair: Martin Head-Gordon</i>		Invited Session 9 <i>Chair: Hiromi Nakai</i>		Invited Session 10 <i>Chair: H. Bernhard Schlegel</i>		Invited Session 11 <i>Chair: Oliver Kühn</i>		Invited Session 12 <i>Chair: Stefan Knippenberg</i>	
13:45	I-071	<i>Jeremy Harvey</i> 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	<i>Kurt Kremer</i> Open systems simulations of macromolecular solutes through adaptive resolutions simulations (AdResS)	I-111	<i>David Clary</i> Quantum dynamical and semi-classical calculations on chemical reactions with application to decomposition of nerve agents	I-121	<i>Benjamin Fingerhut</i> Numerical exact MACGIC-QUAPI simulations of electron transfer dynamics in <i>Drosophila</i> cryptochrome (dCRY)
14:10	I-072	<i>Peter Richard Schreiner</i> 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	<i>Florian Müller-Plathe</i> Multiscale molecular modelling of soft materials: the challenge of dynamics	I-112	<i>Irene Burghardt</i> High-dimensional quantum dynamics of functional organic polymer materials: Coherence, localization, and (dis)order	I-122	<i>Christel Marian</i> TADF efficiencies in coinage-metal coordination complexes and metal-free donor-acceptor systems
14:35	I-073	<i>Leo Radom</i> 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	<i>Christoph Dellago</i> Exploring the mechanism and kinetics of nucleation processes: from crystallization to cavitation	I-113	<i>Roland Mitric</i> Light-induced nonadiabatic dynamics: from isolated molecules to molecular assemblies and light-harvesting nanostructures	I-123	<i>Ilaria Ciofini</i> New tools for the description of excited states of molecular systems in complex environment
15:00	I-074	<i>Yitzhak Apeloig</i> 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	<i>Christine Peter</i> A multiscale simulation perspective on mineralization processes	I-114	<i>Ivano Tavernelli</i> New strategies for non-adiabatic dynamics with trajectories	I-124	<i>Satoshi Maeda</i> Artificial force induced reaction (AFIR) method for automated search of adiabatic and non-adiabatic pathways
15:25	I-075	<i>Kendall Houk</i> 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	<i>Petr Čársky</i> Fourier transform of 1/r on graphical processing units – promising tool for applications in nanolithography	I-105	<i>Alexander Nemukhin</i> Computational modeling of molecular processes in proteins	I-115	<i>Graham Worth</i> Quantum dynamics simulations of photo-excited molecules using the MCTDH method	I-125	<i>Henrik Koch</i> 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 <i>Chair: David Tozer</i>		Contributed Session 2 <i>Chair: Sotiris Xantheas</i>		Contributed Session 3 <i>Chair: Jörn Manz</i>		Contributed Session 4 <i>Chair: William Hase</i>		Contributed Session 5 <i>Chair: Kaori Fukuzawa</i>		Contributed Session 6 <i>Chair: Henk Eshuis</i>	
16:20	C-011	<i>Georg Schreckenbach</i> Modeling of two-dimensional (2D) materials: influence of chemical modifications	C-021	<i>Thomas Kühne</i> The name is bond - hydrogen bond	C-031	<i>Shirin Faraji</i> Utilizing light for repair of light-induced DNA damages: clever mode of action of DNA photolyases	C-041	<i>Manabu Sugimoto</i> First-principles molecular dynamics simulations on ammonia synthesis and decomposition	C-051	<i>Andreas Hauser</i> Carbon nanotubes immersed in superfluid helium: An incomplete flooding due to quantum effects	C-061	<i>Mercedes Alonso</i> Conductance switching in expanded porphyrins through aromaticity and topology changes
16:35	C-012	<i>Lorenzo Maschio</i> Local correlation for crystalline solids: dual basis sets by projection in the reciprocal space	C-022	<i>Tristan Bereau</i> High-throughput screening of drug-membrane thermodynamics	C-032	<i>Oliver Kühn</i> Ultrafast spin-flip dynamics in transition metal complexes triggered by soft X-ray light	C-042	<i>Tetsuya Taketsugu</i> Reaction-path bifurcation analyses based on Valley-Ridge transition and global reaction route mapping	C-052	<i>Raul Alvarez-Idaboy</i> The role of acid-base equilibria in formal hydrogen transfer reactions: uric acid with tryptophanyl radical	C-062	<i>Daniel Aravena</i> Spin-dependent transport and magnetoresistance in metalloporphyrin-based supramolecular wires at room temperature
16:50	C-013	<i>Marek Sierka</i> Density functional theory for periodic systems using density fitting and continuous fast multipole method	C-023	<i>Ragnar Björnsson</i> New insights into nitrogenase: QM/MM broken-symmetry DFT studies of FeMoco and the P-cluster	C-033	<i>Debashree Ghosh</i> Photoprotection mechanism in eumelanin	C-043	<i>Mark Waller</i> Retrosynthesis and reaction prediction with deep neural networks	C-053	<i>Albeiro Restrepo</i> Thermodynamics of the partition of Ibuprofen in a lipid bilayer	C-063	<i>Alexandre Magalhães</i> Catalyzing chemical reactions inside carbon nanotubes
17:05	C-014	<i>Joao B. L. Martins</i> Adsorption of glycerol and dihydroxyacetone on CaO and MgO surfaces	C-024	<i>Alister Page</i> Quantum chemical insights into polymer solvation and Hofmeister effects in aqueous and non-aqueous environments	C-034	<i>Daniel Roca-Sanjuán</i> Chemically-induced excited-state chemistry	C-044	<i>Seiji Mori</i> Graph theory approach in exploration of reaction path networks: Rh(I)BINAP-catalyzed isomerization of allylic amine	C-054	<i>Alessandro Contini</i> Automatization of the Nwat-MMGBSA method to rescore docking results in medium-throughput virtual screening applications	C-064	<i>Michal Straka</i> Theoretical calculations of endohedral fullerenes: from chemical bonding to single-molecule switches
17:20	C-015	<i>Wolfgang Hieringer</i> Electronic structure of molecules at metal surfaces: recent results on organic molecules and coordination compounds	C-025	<i>Olaf Wiest</i> The past, present, and future of Q2MM	C-035	<i>Bo Durbecqj</i> Exploiting excited-state aromaticity for the design of efficient light-driven rotary molecular motors	C-045	<i>Woo Youn Kim</i> Automated searching method for reaction paths using molecular graphs and chemical reaction network	C-055	<i>Przemyslaw Dopieralski</i> Stressed disulfide bonds in alkaline solution	C-065	<i>Matthias Lein</i> Structural and electronic properties of carbon nano-onions
17:35	C-016	<i>Ralf Tonner</i> Explaining organic chemistry at surfaces with energy decomposition analysis	C-026	<i>Dmitry Nerukh</i> Hybrid molecular dynamics - hydrodynamics modelling of liquid solutions: whole virus at atomistic resolution	C-036	<i>László Turi</i> Electronic excited state lifetimes of anionic water clusters: a quantized time correlation function approach	C-046	<i>Anoop Ayyappan</i> Exploring chemical evolution using tabu-search based automated reaction finding algorithm	C-056	<i>Joonkyung Jang</i> Wetting behavior of a surface decorated with periodic pillars	C-066	<i>Juan F. Espinal</i> Nickel effect on the spacing of 002 plane in a graphite-like structure
17:50	C-017	<i>Antti Karttunen</i> Crystal structure prediction of inorganic-organic coordination polymers	C-027	<i>Laurence Leherter</i> Reduced point charge models of proteins - influence of protein-solvent interactions	C-037	<i>Luca De Vico</i> How to control the absorption wavelength of light harvesting complexes	C-047	<i>Wolfgang Quapp</i> Patterns of moving saddle points in catalysis and mechanochemistry	C-057	<i>Petra Imhof</i> Communication in proteins and protein-substrate complexes	C-067	<i>Oscar Lung Wa Chung</i> Mechanistic insights on Ni-catalyzed selective C-O activation & Cu-catalyzed reductive CO ₂ coupling to form oxalate
18:05	C-018	<i>Jon M. Matxain</i> Transition metal doped magnetic Zn ₁₂ S ₁₂ nanoparticles	C-028	<i>Xabier Lopez</i> Insights into the structural toxicity of aluminum with biomolecules, using a computational approach	C-038	<i>Valérie Brenner</i> Excited states deactivation in model proteins chains: Nonadiabatic dynamics simulations and ab initio methods	C-048	<i>Michael Springborg</i> On the theoretical optimization of properties	C-058	<i>Wieslaw Nowak</i> Camphore's and Huperzine's adventures in proteinland	C-068	<i>Amalia I. Poblador Bahamonde</i> Mechanistic investigation on the Pd-catalyzed 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 <i>Chair: Josef Michl</i> <i>Giulia Galli</i> Electrochemistry meets condensed matter physics: first principles simulations of photocatalytic materials										
09:40 – 10:10	COFFEE BREAK											
10:10 – 12:15	Invited Session 13 <i>Chair: Teresa Head-Gordon</i>		Invited Session 14 <i>Chair: Arne Lühchow</i>		Invited Session 15 <i>Chair: Regina de Vivie-Riedle</i>		Invited Session 16 <i>Chair: Attila Császár</i>		Invited Session 17 <i>Chair: Roland Mitric</i>		Invited Session 18 <i>Chair: Christine Peter</i>	
10:10	I-131	<i>Walter Thiel</i> Semiempirical quantum chemistry: methodology and excited-state dynamics	I-141	<i>Ali Alavi</i> Recent developments and applications of full configuration interaction quantum Monte Carlo	I-151	<i>Leticia González</i> Photostability and photodamage in DNA building blocks	I-161	<i>Joel Bowman</i> Many-body potentials for water and protonated water clusters and VSCF/VCI calculations of IR spectra	I-171	<i>Fernando Martin</i> Attochemistry: imaging and controlling electron dynamics in molecules	I-181	<i>Zexing Cao</i> Global simulation of cyanohydrin cleavage by hydroxynitrile lyases
10:35	I-132	<i>Stefan Grimme</i> Applications of the extended tight binding method (GFN-xTB)	I-142	<i>Seiichiro Ten-no</i> Multi-state effective Hamiltonian and size-consistency corrections for stochastic configuration interactions	I-152	<i>Roland Lindh</i> Non-adiabatic chemiluminescent dynamics of the methyl-substituted 1,2-dioxetanes	I-162	<i>Robert Berger</i> What molecules can reveal about fundamental interactions	I-172	<i>Shaul Mukamel</i> Novel multidimensional spectroscopy of conical intersections with X-ray pulses and quantum light	I-182	<i>Tim Clark</i> Metadynamics simulations of G-protein coupled receptors
11:00	I-133	<i>Frank Jensen</i> Developing improved force fields	I-143	<i>Roi Baer</i> Stochastic orbitals for electronic structure and quantum chemistry	I-153	<i>Chantal Daniel</i> Simulation of ultrafast excited state dynamics in transition metal complexes	I-163	<i>R. Benny Gerber</i> Computational vibrational spectroscopy: anharmonic algorithms and determination of 3D structures of biomolecular conformers	I-173	<i>H. Bernhard Schlegel</i> Angular dependence of ionization by short, intense pulses of linear and circularly polarized light	I-183	<i>Markus Meuwly</i> Quantitative atomistic simulations for chemical and biological applications
11:25	I-134	<i>Siewert-Jan Marrink</i> Computational microscopy of (bio) molecular processes	I-144	<i>David Tannor</i> New formulation of quantum mechanics using complex trajectories: application to nonadiabatic transitions and optical excitation	I-154	<i>George Schatz</i> Theories of SERS, TERS, electrochemistry and plasmon-enhanced energy transfer	I-164	<i>Lorenz S. Cederbaum</i> On systems with and without excess energy in environment ICD and other interatomic mechanisms	I-174	<i>Peter Saalfrank</i> Light-driven processes in molecular systems: from photophysics to photochemistry	I-184	<i>Sereina Riniker</i> Replica-exchange enveloping distribution sampling (RE-EDS) to calculate relative binding free energies
11:50	I-135	<i>Jan H. Jensen</i> Using semiempirical methods for fast and automated predictions	I-145	<i>Mark Gordon</i> Dispersion in intermolecular interactions	I-155	<i>Joseph Subotnik</i> Electrochemistry and non-adiabatic dynamics at metal surfaces: the importance of electron-electron correlation	I-165	<i>Sergey Yurchenko</i> Theoretical molecular line lists for atmospheric characterizations of exoplanets	I-175	<i>Peter Knowles</i> On the perturbative computation of ionization energies	I-185	<i>Xuhui Huang</i> 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 <i>Chair: Johan Åqvist</i>		Invited Session 20 <i>Chair: Trygve Helgaker</i>		Industry Session 1 - <i>supported by BASF</i> <i>Chair: Ansgar Schäfer</i>		Invited Session 21 <i>Chair: Markus Meuwly</i>		Invited Session 22 <i>Chair: Odile Eisenstein</i>		Invited Session 23 <i>Chair: Gregory Beran</i>	
13:45	I-191	<i>Teresa Head-Gordon</i> New methods and models for condensed phase simulation	I-201	<i>Don Truhlar</i> Recent progress in density functional theories	IN-1	<i>Peter Deglmann</i> The challenge of chemical thermodynamics and kinetics for real world	I-211	<i>Michele Parrinello</i> Enhanced sampling for chemistry	I-221	<i>Elfi Kraka</i> A comprehensive view on the Claisen rearrangement of chorismate via a new quantum chemical toolbox	I-231	<i>Takeshi Yanai</i> Projector augmented wave method incorporated into Gauss-type atomic orbital based density functional theory
14:10	I-192	<i>Jiali Gao</i> Methods and applications of multistate density functional theory (MSDFT)	I-202	<i>Carlo Adamo</i> Non-empirical double-hybrid functionals: more theoretical constrains, better performances?	IN-2	<i>Christoph Taeschler</i> Mechanistic aspects of high temperature reactions of acetonitrile	I-212	<i>Ulf Ryde</i> Comparison of quantum-mechanical approaches to calculate ligand-binding affinities with free-energy perturbation	I-222	<i>Gabriel Merino</i> Massive search of planar hyper-coordinate carbon atoms	I-232	<i>Claudia Draxl</i> From evaluation of methodology to error bars in computational materials science
14:35	I-193	<i>Modesto Orozco</i> DNA. A fascinating multiscale problem	I-203	<i>Kieron Burke</i> Reliable DFT results for spin-crossover complexes	IN-3	<i>Michael Edmund Beck</i> Digging deep into binding modes in protein-Ligand-complexes by quantum chemistry	I-213	<i>Zhipan Liu</i> Automated reaction pathway sampling using stochastic surface walking method for predicting chemical reactions	I-223	<i>Raghavan B. Sunoj</i> Non-covalent interactions in asymmetric catalysis: a mechanistic voyage from rationalizations to predictions	I-233	<i>Beate Paulus</i> The method of increments applied to weakly bound systems
15:00	I-194	<i>Shina Caroline Lynn Kamerlin</i> Dynamics, flexibility, cooperativity and the evolution of enzyme function	I-204	<i>G Narahari Sastry</i> Cooperativity of non-covalent interactions	IN-4	<i>Marcel Verdonk</i> The use of scoring functions for structure-based drug discovery	I-214	<i>GuanHua Chen</i> Time-dependent density-functional theory for open system and its applications	I-224	<i>Gopalan Rajaraman</i> Are single molecule magnets predictable? Learning from Ab-initio calculations on lanthanide and transition metal molecular-magnets	I-234	<i>Krzysztof Szalewicz</i> Physics-based intermolecular potentials for material design
15:25	I-195	<i>Helmut Grubmüller</i> Towards a mechanistic understanding of ribosomal function	I-205	<i>David Sherrill</i> Large datasets for benchmarking noncovalent interactions	IN-5	<i>Thomas Fox</i> Free energy calculations in drug design	I-215	Michele Pavanello Real and imaginary-time electron dynamics of open quantum subsystems	I-225	<i>Laura Gagliardi</i> Computationally guided discovery of metal-decorated metal-organic frameworks active for catalysis	I-235	<i>WanZhen Liang</i> 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 <i>Chair: Kieron Burke</i>		Contributed Session 8 <i>Chair: Max Holthausen</i>		Industry Session 2 - <i>supported by BASF</i> <i>Chair: Robert Franke</i>		Contributed Session 9 <i>Chair: Daniel Escudero</i>		Contributed Session 10 <i>Chair: Woo Youn Kim</i>		Contributed Session 11 <i>Chair: Iris Antes</i>	
16:20	C-071	Mario Piris NOF-MP2: a global method for the electron correlation	C-081	Andrey Rogachev Trianionic corannulene: tuning 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– <i>supported by The Journal of Physical Chemistry</i>											

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 <i>Chair: Peter Richard Schreiner</i> Pavel Hobza Noncovalent interactions: theory and applications										
09:40 10:10	COFFEE BREAK											
10:10 12:15	Invited Session 24 <i>Chair: Mark Gordon</i>		Invited Session 25 <i>Chair: Gernot Frenking</i>		Invited Session 26 <i>Chair: Guan Hua Chen</i>		Invited Session 27 <i>Chair: Martin Kaupp</i>		Invited Session 28 <i>Chair: Qiang Cui</i>		Invited Session 29 <i>Chair: Dominika Zgid</i>	
10:10	I-241	<i>Alán Aspuru-Guzik</i> 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	<i>Michele Ceriotti</i> 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 Izaquirre 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	<i>Markus Reiher</i> 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 TiO ₂ 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	<i>Matthias Scheffler</i> 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	<i>Gregory Voth</i> 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 <i>Chair: So Hirata</i> <i>Hiroshi Nakatsuji</i> 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 <i>Chair: Asbjörn Burów</i>		Invited Session 31 <i>Chair: Manuel Yáñez</i>		Invited Session 32 <i>Chair: Luca Frediani</i>		Invited Session 33 <i>Chair: Christof Hättig</i>		Invited Session 34 <i>Chair: Bogumil Jeziorski</i>		Invited Session 35 <i>Chair: Zexing Cao</i>	
10:10	I-301	<i>Filipp Furche</i> Recent developments in random phase approximation methods	I-311	<i>Josef Michl</i> Oligosilanes: intuitive understanding of σ delocalization in loose and localization in tight helical conformations	I-321	<i>Chiara Cappelli</i> A fully polarizable embedding model for molecular spectroscopy of aqueous solutions	I-331	<i>Anna Krylov</i> Visualizing the contributions of virtual states to two-photon absorption cross-sections	I-341	<i>Rodney J. Bartlett</i> Quantitative molecular orbital theory	I-351	<i>Pedro Fernandes</i> Nanosecond-timescale conformational dynamics of enzymes, and its impact on reaction rates
10:35	I-302	<i>Axel Becke</i> Vertical excitation energies from the adiabatic connection	I-312	<i>Gernot Frenking</i> Aspects of chemical bonding	I-322	<i>Jacob Kongsted</i> Excited states in complex systems through polarizable (density) embedding	I-332	<i>Xiaosong Li</i> Two-component non-collinear time-dependent spin density functional theory for electronic dynamics and excited state calculations	I-342	<i>Andreas Köhn</i> Applications of interrenally contracted multireference coupled-cluster theory	I-352	<i>Yiqin Gao</i> Computer simulations of chemical reactions in solution
11:00	I-303	<i>Eunji Sim</i> Reliable DFT results with density correction	I-313	<i>Marco Nascimento</i> Are one-electron bonds any different from standard two-electrons covalent bonds?	I-323	<i>Lyudmila Slipchenko</i> Polarizable embedding and beyond: modeling photoactive proteins with the effective fragment potential method	I-333	<i>Andreas Dreuw</i> Algebraic diagrammatic construction - a versatile approach to excited states, ionization potentials and electron affinities	I-343	<i>Shuhua Li</i> Advances in Electronic Structure Methods for Strongly Correlated Systems and Condensed Phase Systems	I-353	<i>Young Min Rhee</i> Simulating photo-excited dynamics of biological complexes: overcoming present challenges with interpolated potentials
11:25	I-304	<i>Andreas Görling</i> Density-functional methods with the accuracy and wide applicability of high-level multi-reference approaches	I-314	<i>Julia Contreras-García</i> A new model for reference densities - really getting rid of interactions	I-324	<i>Fred Manby</i> Multiscale embedding methods for accurate quantum chemistry of complex systems	I-334	<i>Spiridoula Matsika</i> Theoretical studies of the interaction of uracil with low energy electrons	I-344	<i>Jiri Pittner</i> DMRG-externally-corrected local pair natural orbital based coupled cluster method	I-354	<i>Carmay Lim</i> How native and alien metal cations bind ATP
11:50	I-305	<i>Paul Ayers</i> Variational principle for partitioning molecules into atomic contributions	I-315	<i>Russell J. Boyd</i> Insight into hydrogen-bonded clusters and noncovalent interactions from changes in atomic energies	I-325	<i>Kurt V. Mikkelsen</i> Exploitation of solar energy	I-335	<i>John Herbert</i> First-principles exciton models, with application to singlet fission	I-345	<i>Ove Christiansen</i> Tensor decomposition and coupled cluster theory	I-355	<i>David Smith</i> 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 <i>Chair: Jiali Gao</i>		Invited Session 37 <i>Chair: Filipp Furche</i>		Invited Session 38 <i>Chair: Julien Toulouse</i>		Invited Session 39 <i>Chair: Francesco Aquilante</i>		Invited Session 40 <i>Chair: Andreas Dreuw</i>		Invited Session 41 <i>Chair: Brian Yates</i>	
13:45	I-361	<i>Richard Henchman</i> Theory for the entropy of liquid mixtures of flexible molecules	I-371	<i>Marcel Noojien</i> Towards a local coupled cluster theory for solids	I-381	<i>So Hirata</i> Many-body Green's function theory: algebraic recursions, linked- and irreducible-diagram theorems, and general-order algorithms	I-391	<i>Toru Shiozaki</i> On-the-fly CASPT2 surface hopping dynamics	I-401	<i>Patrick Norman</i> Response theory techniques to address X-ray spectroscopies	I-411	<i>Igor Alabugin</i> Reinventing cycloaromatization reactions: the diradical /zwitterion dichotomy
14:10	I-362	<i>Johan Åqvist</i> Entropy and enzyme catalysis	I-372	<i>Georg Kresse</i> The relation between the random phase approximation and GW and analytic forces for the RPA	I-382	<i>Dominika Zgid</i> Green's function embedding methods	I-392	<i>David Tew</i> Quantum dynamics on accurate electronic potentials	I-402	<i>Daniel Crawford</i> Streamlining coupled cluster response theory	I-412	<i>Miroslav Urban</i> DFT study of the Au-C bond formation in gold implanted polyethylene
14:35	I-363	<i>Qiang Cui</i> Understanding metalloenzyme catalysis with QM/MM free energy simulations	I-373	<i>Silke Biermann</i> Electronic structure calculations for correlated electron materials: a dynamical mean field perspective	I-383	<i>Denis Jacquemin</i> Is BSE/GW an effective method for modeling optical spectra of molecules?	I-393	<i>Yuki Kurashige</i> Ab initio modeling of inter-molecular electronic transition processes in molecular aggregates	I-403	<i>Benoît Champagne</i> Towards investigating the optical properties of molecular and ionic crystals using multi-scale approaches	I-413	<i>Attila Császár</i> A structural molecules
15:00	I-364	<i>Pavel Jungwirth</i> Cell penetration and membrane fusion: two sides of the same coin	I-374	<i>Volker Blum</i> Affordable high numerical accuracy for large molecules and materials from numeric atom-centered basis functions	I-384	<i>Lucia Reining</i> Quasi-particles and satellites from a direct approach to the calculation of many-body Green's functions	I-394	<i>Hans Jørgen Aagaard Jensen</i> Open-shell MC-srDFT - a new way to describe high-spin, low-spin, intermediate spin states and more	I-404	<i>Sonia Coriani</i> Developing theoretical "beam-lines" for modern experiments	I-414	<i>Annia Galano</i> The role of acid-base equilibria in the antioxidant and pro-oxidant activity of phenolic compounds
15:25	I-365	<i>Gerhard Hummer</i> Molecular simulations of lipid membrane sensing and remodeling dynamics	I-375	<i>Gregory Beran</i> Ab initio molecular crystallography: Aiding and abetting experiment	I-385	<i>Wim Klopper</i> Using the GW and Bethe-Salpeter methods in molecular quantum chemistry	I-395	<i>Piotr Piecuch</i> Stochastic CC(P;Q) theory: converging high-level coupled-cluster energetics by Monte Carlo sampling and moment expansions	I-405	<i>Antonio Rizzo</i> Electronic nonlinear spectroscopies: recent contributions of theory and computational science	I-415	<i>Munir Skaf</i> 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 <i>Chair: David Tew</i>	Contributed Session 13 <i>Chair: Wolfgang Domcke</i>	Contributed Session 14 <i>Chair: Andy Teale</i>	Contributed Session 15 <i>Chair: Reinhold Fink</i>	Contributed Session 16 <i>Chair: Tanya K. Todorova</i>	Contributed Session 17 <i>Chair: Marco Nascimento</i>
16:20	C-121 <i>Jan M.L. Martin</i> Explicitly correlated benchmark study on water clusters: The right answer for the right reason?	C-131 <i>Nick Mayhall</i> Multiexcitons and strong correlation via single-excitation wavefunctions: applications and future directions	C-141 <i>Stella Stopkowicz</i> Accurate treatment for ground and excited states of atoms and molecules in strong magnetic fields	C-151 <i>Martin Kaupp</i> Mixed valency and local hybrid functionals	C-161 <i>Mark Iron</i> Computational insights into sulphur isotopic fractionation in carbonate-associated sulphate	C-171 <i>José Enrique Barquera-Lozada</i> Aromaticity from the point of view of the vorticity of the current density tensor
16:35	C-122 <i>Ricardo Mata</i> GoBench: a joint initiative for experimental benchmarking of quantum chemical methods	C-132 <i>Remco Havenith</i> The computation of dielectric constants	C-142 <i>Sandra Luber</i> Recent advances in theoretical spectroscopy from ab initio molecular dynamics	C-152 <i>Lars Goerigk</i> Double-hybrid density functionals: is there anything new to tell?	C-162 <i>Silvia Simon</i> Tailoring resonance assisted hydrogen bonds	C-172 <i>Fabio Pichierri</i> Cesium cation- π interactions: DFT and QTAIM studies
16:50	C-123 <i>Peter Nagy</i> Approaching CCSD(T)/CBS energies for large molecules with the linear-scaling local natural orbital CCSD(T) method	C-133 <i>Andrzej L. Sobolewski</i> Organic photovoltaics with p-f-n junctions: computational study of ferroelectric columnar molecular clusters	C-143 <i>Malgorzata Biczysko</i> Anharmonic effects on vibrational spectra intensities: infrared, Raman, vibrational circular dichroism, and Raman optical activity	C-153 <i>Sergei Vyboishchikov</i> Exchange-Correlation Potentials and Energy Densities in Spherically Confined Atoms	C-163 <i>Ulrike Salzner</i> Effect of biradical character of organic molecules on Opto electronic properties	C-173 <i>András Stirling</i> Hypervalency and reactivity from Wannier orbitals
17:05	C-124 <i>Graham Fletcher</i> Large-scale valence bond applications: excitons and transition metal complexes	C-134 <i>Thomas Koerzdoerfer</i> Accurate ionization potentials, electron affinities, and photoelectron spectra of molecules from first principles	C-144 <i>Takeshi Iwasa</i> Infrared absorption spectroscopy beyond the dipole approximation based on the multipolar Hamiltonian: Theory and application	C-154 <i>Arindam Chakraborty</i> Linked-cluster formulation of screened electron-hole interaction from explicitly-correlated geminal functions without using unoccupied states	C-164 <i>Hong-Xing Zhang</i> Computationally driven design of efficient photosensitizer for dye-sensitized solar cell applications	C-174 <i>Leonardo Belpassi</i> Charge-displacement analysis: a simple tool to reveal charge transfer effects throughout the whole periodic table
17:20	C-125 <i>Jean-Philip Piquemal</i> Scalable polarizable molecular dynamics using Tinker-HP: millions of atoms on thousands of cores	C-135 <i>Emanuele Coccia</i> Dissipation and dephasing for molecules close to plasmonic nanoparticles: an ab initio approach	C-145 <i>Franco Egidi</i> Toward the accurate simulation of vibrationally-resolved spectra for spin-forbidden transitions	C-155 <i>István Mayer</i> Local spins	C-165 <i>Martial Boggio-Pasqua</i> Computational studies of the photoswitching mechanisms in photochromic ruthenium complexes	C-175 <i>Apostolos Kalemios</i> The nature of the chemical bond in Be containing molecules: Be 2^{+} , Be $^{+}$, Be 3 , BeO $^{+}$, BeOBe $^{+}$, Be $^{+}$
17:35	C-126 <i>Joonsuk Huh</i> Vibronic boson sampling	C-136 <i>Robert Góra</i> Microhydration induces qualitative changes in the photochemistry of biomolecular building blocks	C-146 <i>Sergei Ivanov</i> Nuclear correlation effects in X-ray spectroscopy from a time-domain perspective	C-156 <i>Fan Wang</i> Spin-orbit coupling effects of open-shell systems with coupled-cluster theory	C-166 <i>Aurélien Perrier</i> Photosensitizing properties of functionalized thiolate-protected gold nanoclusters: insights from theory	C-176 <i>David Wilson</i> Theoretical investigation of a strong cis-effect in an imidazole-imidazolium substituted alkene
17:50	C-127 <i>Luca Frediani</i> PCMSolver: a modern, modular approach to include solvation in any quantum chemistry code	C-137 <i>Isabelle Navizet</i> Role of the environment in bioluminescence emission: QM/MM study	C-147 <i>Stepan Sklenak</i> DFT calculations of NMR parameters of framework and extra-framework atoms in silicon-rich zeolites	C-157 <i>Mikael P. Johansson</i> Can spin-state energetics of transition metal complexes be accurate at single reference level?	C-167 <i>David Henry</i> Modifying the reactivity of gallium nanoclusters with ligands	C-177 <i>Ignacy Cukrowski</i> Fragment attributed molecular system energy change (FAMSEC) in the study of interactions and molecular stability
18:05	C-128 <i>Sebastian Höfener</i> Combining frozen-density embedding with the conductor-like screening model using Lagrangian techniques	C-138 <i>Stefan Knippenberg</i> Investigation of optical probes for membrane phase recognition	C-148 <i>Alfonso Hernández-Laguna</i> Elastic behavior of White Micas solid solutions as a function of the pressure	C-158 <i>Ran Friedman</i> Specific ion interactions with biomolecules: molecular dynamics simulations and energy decomposition analysis	C-168 <i>Thibaud Étienne</i> Orbital relaxation and electronic transitions - what is the nature of Handy's Z-vector?	C-178 <i>Hugo Gattuso</i> 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 <i>Chair: David Sherrill</i>	
09:00 09:40	PL-9	<i>Francesco Evangelista</i> Multireference coupled cluster theory, infinities and renormalization
09:40 10:20	PL-10	<i>Johannes Neugebauer</i> 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 <i>Chair: Walter Thiel</i>	
10:50 11:30	PL-11	<i>Ursula Roethlisberger</i> Next generation first-principles based multiscale simulations: computational chemistry meets artificial intelligence
11:30 12:10	PL-12	<i>Frank Neese</i> Wavefunction based correlation methods for large molecules: recent developments, applications and limitations
12:10 12:50	CLOSING CEREMONY AND POSTER AWARDS	



POSTER SESSIONS



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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-methylenadamantane
Yuji Naruse, Japan
- PO1-4** Radiative association of ^{36}Ar and ^{38}Ar 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 $[\text{Re}(\text{CO})_x]^+/\text{CH}_4$ ($x=0\text{X}3$) 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 $\text{Li}_{12}\text{F}_{13}$ - 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

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- 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 naphthalene
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 α aminophosphonates 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 CO₂ fixation by monoethanolamine
Maneepon 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 CO₂ capture in swing adsorption processes
Hector Prats Garcia, Spain
- PO1-51** Ni-phosphine bond strengthening through 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

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- 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 multireference approach
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

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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 CO₂ disproportionation and hydrogenation
Lisa Roy, Germany
- PO1-96** Molecular dynamics simulation reveals how phosphorylation of tyrosine 26 of PGAM1 upregulate glycolysis
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- 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

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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 $[C_{20}X_{20}]^-$, $[C_{20}X_{20}]^{-2}$, $[Si_{20}F_{20}]^-$, $[Si_{20}F_{20}]^{-2}$ (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** CO₂ 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

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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 CO₂ 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
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- 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 Froushani, Australia
- PO1-152** On-the-fly kinetic Monte Carlo based on global reaction route mapping
Izaak 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
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- 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
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- 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

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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 Götze, 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 Ce_{1-x}O₂(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
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Xu Zhang, China

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Johannes Dietschreit, Germany

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Fabijan Pavosevic, United States

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Sergi Ruiz-Barragan, Germany

Site-occupation embedding theory using Bethe ansatz local density approximation

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

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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

Name Badges

During the congress, please wear your name badge at all times. The badge is your entrance ticket to the session halls.

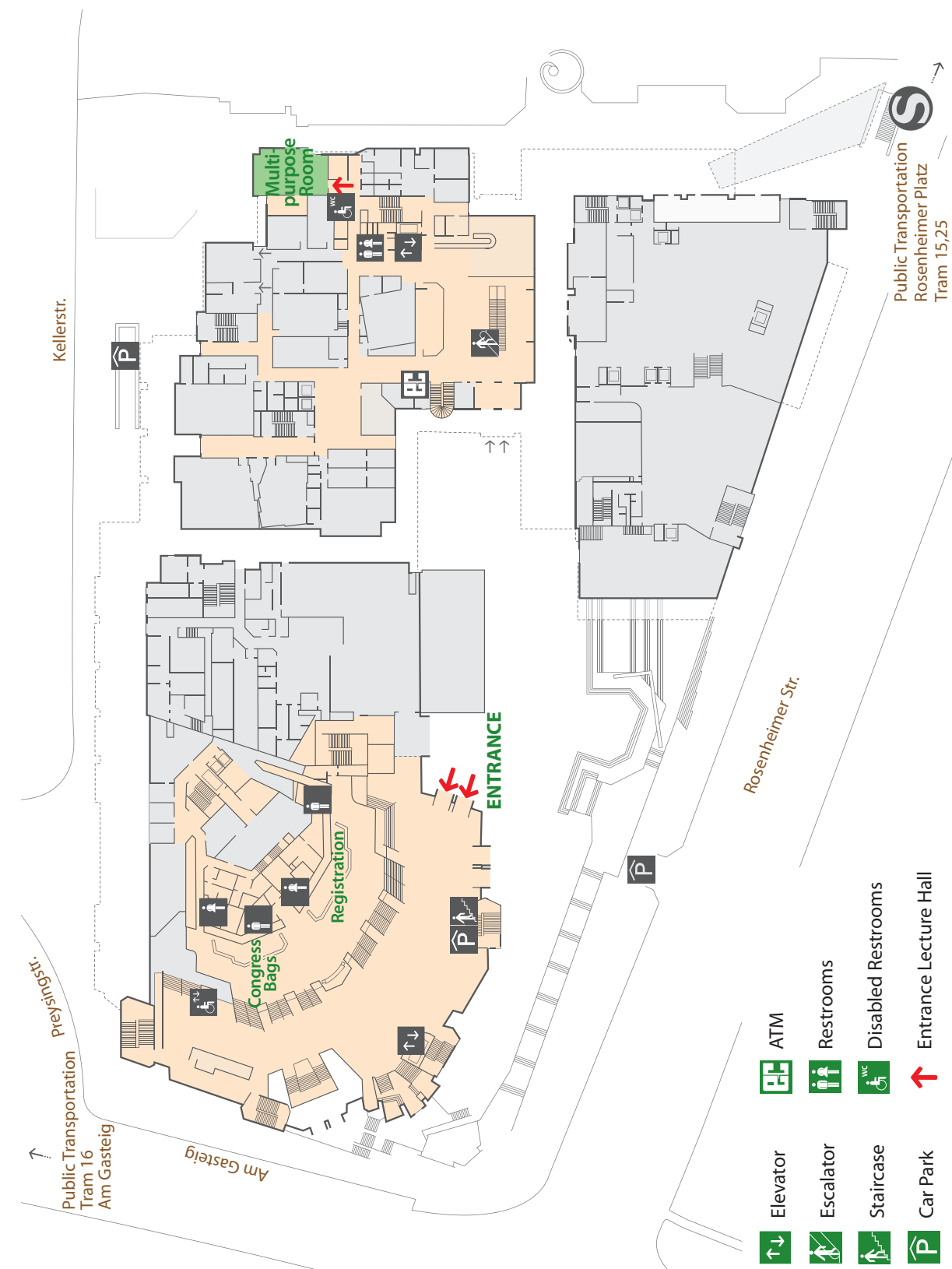
Lectures

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

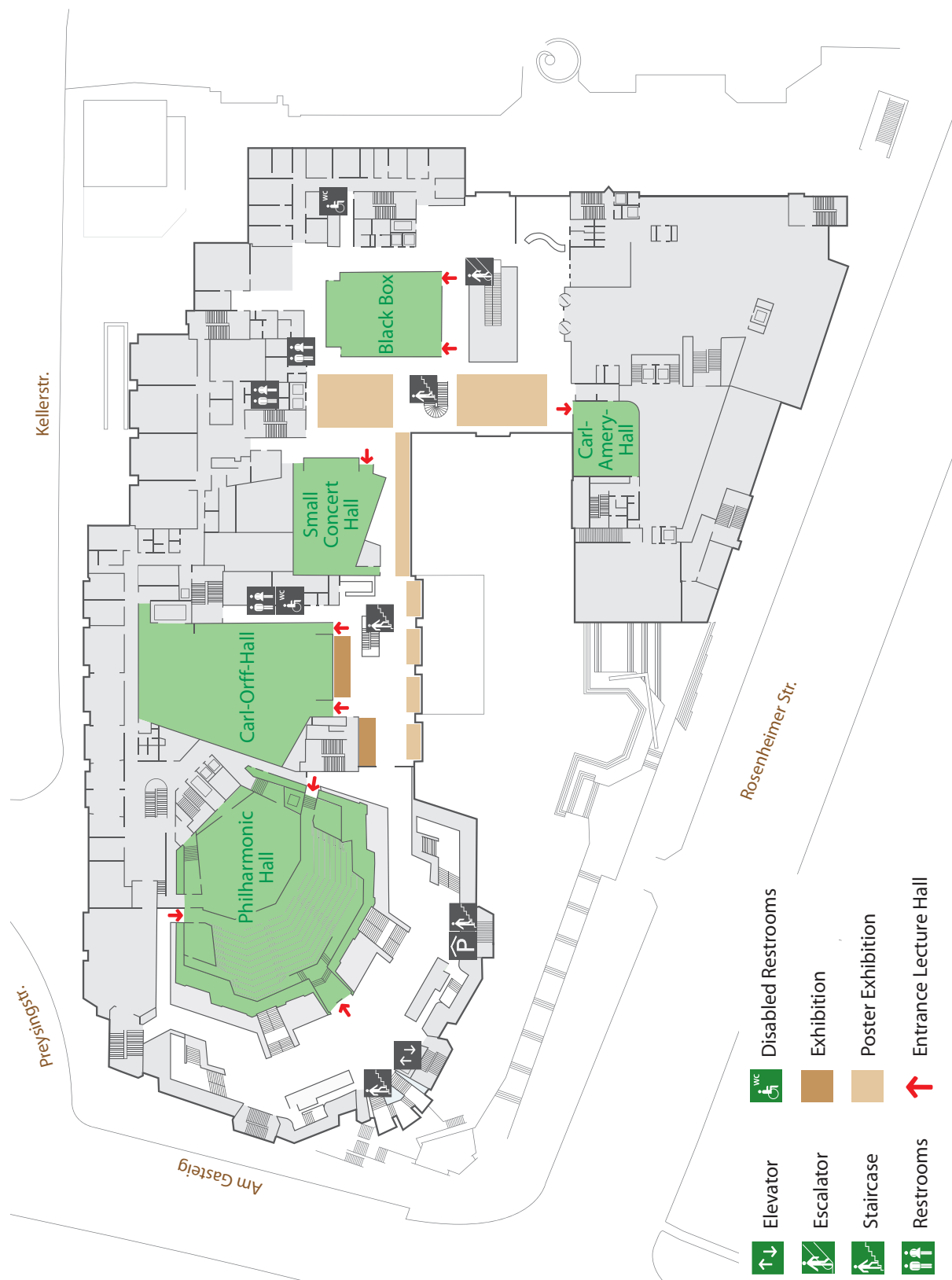
Poster Awards

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.



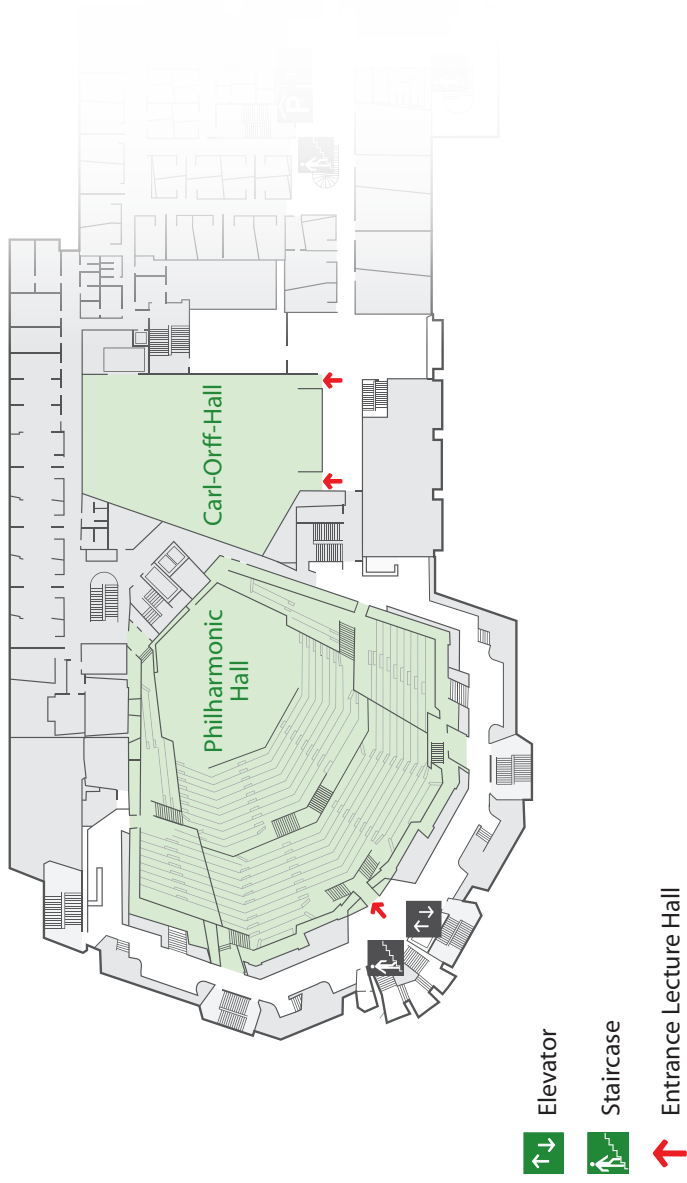


Floor Plan – First Floor





Floor Plan – Second Floor





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Zhu J.	PO1-49
Ziebarth B.	IN-10
Zins E.-L.	PO1-49
Zipse H.	PO2-141, PO2-71
Zlatař M.	PO2-217
Zobel P.	PO2-113
Zöllner M.S.	PO2-251, PO2-280

Żuchowski P.	PO1-133
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