PROGRAM SCHEDULE

CONGRESS OF THE INTERNATIONAL SOCIETY OF THEORETICAL CHEMICAL PHYSICS 2016 CONFERENCE
ALERUS CENTER, 1200 South 42nd Street, Grand Forks, ND, USA
JULY 17-22, 2016

SUNDAY, JULY 17

BALLROOM 5

3:00pm-9:00pm **Registration**

4:00pm-5:00pm **Opening Remarks**

5:00pm-6:00pm **Plenary I** **Chair: M. Hoffmann**
Andreas Savin (CNRS; University of Paris - Sorbonne)
''Multireference Density Functional Theory"

6:00pm-7:00pm **AFTERNOON SESSION** **Chair: P. Gill**
Mixed I
Kenneth Ruud (University of Tromsø)
"Molecular Response Properties in the Relativistic Domain"

Katarzyna Pernal (Lodz University of Technology)
"*Reduced Density Matrix Embedding"*

7:15pm-9:15pm **Welcome Reception**

MONDAY, JULY 18

7:30am-6:00pm **Conference Registration**

8:00am-9:30am **MORNING SESSION A**
BALLROOM 5 **Electronic Structure IA** **Chair: P. Piecuch**
Paul Ayers (McMaster University)
"Geminals-Based Approaches for Strongly Correlated Systems with Open Shells"

Garnet Chan (Princeton University)
"Periodic Quantum Chemistry"

Mihály Kállay (Budapest University of Technology and Economics)
"*Efficient Fragmentation-Based Linear-Scaling CCSD(T) Methods"*

ORIOLE ROOM 2 **Complex Systems IA** **Chair: J. Gao**
Jiali Gao (University of Minnesota)

Heather Kulik (Massachusetts Institute of Technology)
"Quantifying Electronic Effects in Enzyme Active Sites"

Yasuteru Shigeta (University of Tsukuba)
"Efficient Conformational Search Methods for Protein Folding Problems"

PHEASANT ROOM 3 **DFT Subsystems IA** **Chair: J. Neugebauer**
Tomasz Wesolowski (University of Geneva)
"Recent Progress in Density Embedding Theory and its Applications?"

Michele Pavanello (Rutgers University)
"Embedding Ground and Excited States in Real and Imaginary Time"

Claudia Filippi (University of Twente)
"Multiscale Modeling for Excited States: Capturing Polarization in Biomolecules"

9:30am-10:00am **Coffee Break** 

10:00am-11:00am *BALLROOM 5*

Plenary II **Chair: P. Surjan**

Debashis Mukherjee (Indian Association for the Cultivation of Science)
"A Survey of the Unitary Group Adapted MRCC and MRPT Theories: SU vs SS Approaches"

11:00am-12:30pm

MORNING SESSION B

BALLROOM 5

Electronic Structure IB **Chair: G. Scuseria**

Andreas Köhn (University of Stuttgart)
"Internally Contracted Multireference Coupled-Cluster Theory"

Ron Shepard (Argonne National Laboratory)
"Recent Developments with the Graphically Contracted Function Electronic Structure Method"

Ali Alavi (University of Cambridge)
"Advances in Large scale CASSCF and Multi-reference Perturbation Theory using Full CI Quantum Monte"

ORIOLE ROOM 2

Complex Systems IB **Chair: J. Gao**

Xiaosong Li (University of Washington)
"Non-collinear Spin in Quantum Chemistry"

Irene Burghardt (Goethe University Frankfurt)
''High-dimensional Quantum Dynamics of Functional Organic Polymer Materials: Coherence and Correlations at the Nanoscale"

John Herbert (Ohio State University)
"*Symmetry-Adapted Perturbation Theory for Many-Body Systems"*

PHEASANT ROOM 3

DFT Subsystems IB **Chair: L. Visscher**

Weitao Yang (Duke University)
"Embedding of Two-Electron Subsystems within DFT for Ground and Excited States"

Piotr de Silva (Massachusetts Institute of Technology)
''Many-Pair Expansion: A Systematically Improvable Correction Scheme for Including Strong and Long-Range Correlations in DFT"

Kieron Burke (University of California-Irvine)
"A Foolish Consistency is the Hobgoblin of Little Minds"

2:00pm-3:30pm

AFTERNOON SESSION A

BALLROOM 5

Molecular Properties IA **Chair: T. Helgaker**

Timo Fleig, (University of Paul Sabatier Toulouse)
"Atoms and Molecules as Laboratories for Probing Physics Beyond the Standard Model"

Peter Schmelcher, (University of Hamburg)
"Ultralong-Range Molecules: Binding, Properties and Control with External Fields"

Erik Tellgren, (University of Oslo)
"Non-perturbative Treatment of Molecules in Non-uniform Magnetic Fields"

ORIOLE ROOM 2

Complex Systems IIA **Chair: N. Ananth**

Donald Truhlar, (University of Minnesota)
"The Quest for a Universal Density Functional for Treating Complex Systems"

Neepa Maitra (Hunter College CUNY)
"Non-Adiabatic Dynamics in Strong Fields: Enhanced Ionization"

Robert Distasio (Cornell University)
"The Dipole Polarizability of a Condensed-Phase Water Molecule"

PHEASANT ROOM 3 **DFT Subsystems IIA** **Chair: ~~D. Crawford~~**

Adam Wasserman (Purdue University)
"Fixing Errors of Approximate XC-functionals with Partition Density Functional Theory"

Jason Goodpaster (University of Minnesota)
"Quantum Embedding Methods for Wave-Function-in-Density Functional Theory: Projection Based Embedding and Density Matrix Embedding Theory"

Mark Hoffmann (University of North Dakota)
"Chemical Bonds in Subsystem Embedding Theory with External Orbital Orthogonality"

3:30pm-4:00pm **Coffee Break** 

4:00pm-5:00pm **Plenary III** **Chair: K. Pernal**
BALLROOM 5
Kim Baldridge (Tianjin University and ETH Zürich)
"Structure–Property Relationships of Curved Aromatic Materials from First Principles"

5:00pm-6:30pm **AFTERNOON SESSION B**
BALLROOM 5 **Molecular Properties IB** **Chair: T. Fleig**
Filipp Furche, (University of California, Irvine)
"Unphysical Divergences in Approximate Response Theory"

Filip Pawlowski, (Aarhus University)
"Why Cluster Perturbation Theory and Not Coupled Cluster Theory?"

Andy Teale (University of Nottingham)
"Current-Density-Functional Theory: Progress and Challenges"

ORIOLE ROOM 2 **Complex Systems IIB** **Chair: N. Ananth**
Ryan Steele, (University of Utah)
"Vibrational Signatures of Electronic Properties in Energy and Biology"

Jiri Vanicek, (Ecole Polytechnique Federale de Lausanne)
"On-the-fly Ab Initio Semiclassical Dynamics for Computing Vibrationally Resolved Electronic Spectra"

Mark Tuckerman, (New York University)
"Exploration and Generation of Free Energy Landscapes of Molecular Crystals and Oligopeptides"

PHEASANT ROOM 3 **DFT Subsystems IIB** **Chair: C. Filippi**
Lyudmila Slipchenko, (Purdue University)
"BioEFP: Polarizable Embedding in Biological Systems"

Debashree Ghosh, (National Chemical Laboratory)
"Hybrid Quantum Mechanical / Effective Fragment Potential Methods: Towards Accurate Solvatochromic Shifts in Biological Medium"

Chen Huang (Florida State University)
"Patching Exchange-Correlation Potential in Density Functional Theory"

6:30pm-8:30pm **Poster Session I**
BALLROOM 4

TUESDAY, JULY 19

8:00am-9:30am **MORNING SESSION A**
BALLROOM 5 **Electronic Structure IIA** **Chair: H. Nakai**
Hans Lischka, (Tianjin University)
"The Polyradical Character of Kekulé and Non-Kekulé Structures of Polyaromatic Hydrocarbons"

Monika Musiał, (University of Silesia)
"Novel Treatment of the High-Multiplicity States with the EOM Method and RHF Reference Function"

Gustavo Scuseria, (Rice University)
"New Vistas on the Strong Correlation Problem"

ORIOLE ROOM 2 **DFT Subsystems IIIA** **Chair: G. Chan**

Thomas Miller, (California Institute of Technology)
"Quantum Embedding Methods for the Simulation of Condensed-Phase Systems"

Gang Lu, (California State University Northridge)
"Density-Based Embedding for QM/MM Modeling of Metals"

Johannes Neugebauer, (University of Muenster)
"Excited States in Protein-Pigment Complexes"

PHEASANT ROOM 3 **Chemical Insights IA** **Chair: T. Rocha-Rinza**

Pedro Salvador, (Universitat de Girona)
"One- and Two-Center Physical Space Decomposition of the Kohn-Sham Density Functional Theory Energy"

Carlos Cárdenas (University of Chile)
"Chemical Response Functions in Degenerate States and Extended Systems"

Laurent Joubert, (University of Rouen)
"Unraveling Charge Transfer Processes with the Quantum Theory of Atoms-in-Molecules"

9:30am-10:00am **Coffee Break**

10:00am-11:00am **Plenary IV** **Chair: H. Nakatsuji**
BALLROOM 5 **Henry F. Schaefer III** (University of Georgia)

11:00am-12:30pm **MORNING SESSION B**
BALLROOM 5 **Electronic Structure IIB** **Chair: M. Kállay**

Ágnes Szabados, (Eötvös Loránd University)
"Novel Orthogonalization Algorithms and Their Use in Electronic Structure Theory"

Péter Surján, (Eötvös Loránd University)
"Convergence Enhancement in Rayleigh-Schrodinger Perturbation Theory: Quantum Chemical Applications"

Masahiro Ehara, (Institute for Molecular Science)
"Recent Progress in CAP/SAC-CI Method for Locating Resonance States"

ORIOLE ROOM 2 **DFT Subsystems IIIB** **Chair: M. Reiher**

Gerald Knizia, (Pennsylvania University)

Andre Severo Pereira Gomes, (Laboratoire de Physique des Lasers Atomes et Molécules (PhLAM) CNRS)
"Frozen-density Embedding Calculation of Second-order Magnetic Properties in the Relativistic Framework"

Florian Libisch, (Vienna University of Technology)
"Embedding Approaches for Bulk Systems Using Projector-Augmented Waves"

PHEASANT ROOM 3 **Chemical Insights IB** **Chair: E. Matito**

Tomás Rocha-Rinza, (Universidad Nacional Autónoma de México)
"Some Developments of Quantum Chemical Topology and Their Applications to the Study of H-Bond In Ground and Excited States"

Ida-Marie Høyvik, (NTNU)

"Connecting the Shape of Localized Hartree-Fock Orbitals to Electronic Properties of the Molecular System"

Benjamin Janesko, (Texas Christian University)
"The Electron Delocalization Range"

2:00pm-3:30pm **AFTERNOON SESSION A**

BALLROOM 5 **Electronic Structure IIIA** **Chair: P. Ayers**

Benjamin Levine, (Michigan State University)
"Multireference Quantum Chemistry and Conical Intersections at the Nanoscale"

Hiroshi Nakatsuji, (Quantum Chemistry Research Institute)
"Formulation of the Free-Complement Valence Bond Method for Solving the Schrödinger Equation of Atoms and Molecules"

Seiichiro Ten-no, (Kobe University)
"Massively Parallel Calculation of Accurate Electronic Structures"

ORIOLE ROOM 2 **DFT Subsystems IVA** **Chair: T. Wesolowski**

Octavio Roncero, (Instituto Fisica Fundamental, CSIC)
"Density-Difference-Driven Optimized Embedding Potential Method to Study the Spectroscopy of Br_2 in Water Clusters"

Caroline Krauter, (Princeton University)
"Embedded Correlated Wavefunction Methods and their Application to Plasmon-Enhanced Heterogeneous Catalysis"

Rustam Khaliullin, (McGill University)
"Fast Linear Scaling Density Functional Theory Based on Local Seamlessly Interconnected Orbital Domains"

PHEASANT ROOM 3 **Molecular Properties IIA** **Chair: S. Stopkowicz**

Benoit Champagne, (University of Namur)
"First-Principles Numerical Simulations for Simulating and Interpreting Sum Frequency Generation Spectra of Functionalized Surfaces"

Chiara Cappelli, (Scuola Normale Superiore)
"Modeling Molecular Properties and Spectroscopies of Strongly Interacting Solute-Solvent Systems"

Christian Ochsenfeld, (University of Munich)
"Linear- and Sublinear-Scaling Calculation of Properties for Large Molecular Systems"

3:30pm-4:00pm **Coffee Break** 

4:00pm-5:00pm **Plenary V** **Chair: D. Truhlar**

BALLROOM 5 **Benedetta Mennucci**, (University of Pisa)
"Ab Initio Simulation of the Optical Spectroscopy of Multichromophoric Systems"

5:00pm-6:30pm ***AFTERNOON SESSION B***

BALLROOM 5 **Electronic Structure IIIB** **Chair: H. F. Schaefer III**

Hiromi Nakai, (Waseda University, CREST, and Kyoto University)
"Linear-Scaling Method for Nonlocal Excited States by Dynamical Polarizability Computations"

Wei Li, (Nanjing University)
"Cluster-In-Molecule and Generalized Energy-Based Fragmentation Coupled Cluster for Large Systems"

ORIOLE ROOM 2 **Mixed II** **Chair: G. Aucar**

Krishnan Raghavachari, (Indiana University)
"Connectivity-Based Hierarchy to Eliminate Systematic Errors: CCSD(T)-Quality Reaction Enthalpies at MP2 or DFT-Cost"

Wim Klopper, (Karlsruhe Institute of Technology)
"Explicitly Correlated Wave Functions in the Random-Phase Approximation to the Correlation Energy"

Peter Gill, (Australian National University)
"MP2 Energies, By Jove!"

PHEASANT ROOM 3 **Molecular Properties IIB** **Chair: P. Schmelcher**
Svetlana Berdyugina, (Kiepenheuer Institut für Sonnenphysik)
"*Molecules as Diagnostics of Cosmic Magnetic Fields and Exoplanets"*

Anand Thirumalai, (University of Oslo)
"Forays into the Unknown: Atoms and Molecules in Magnetised Compact Objects"

Stella Stopkowicz, (Universität Mainz)
"Coupled-Cluster Theory for Atoms and Molecules in Strong Magnetic Fields"

6:30pm-8:30pm **Poster Session II**
BALLROOM 4

WEDNESDAY, JULY 20

8:00am-9:30am **MORNING SESSION A**
BALLROOM 5 **Per-Olov Löwdin IA** **Chair: R. Bartlett**
Anna Krylov, (USC)
"Complex-Variable Approaches for Metastable Electronic States"

Erkki Brändas, (Uppsala University)
"Per-Olov Löwdin: The Father of Quantum Chemistry"

ORIOLE ROOM 2 **Emerging Methods IA** **Chair: E. Valeev**
Francesco Evangelista, (Emory University)

Eric Neuscamman, (University of California-Berkeley)
"Exciting Developments in Quantum Monte Carlo"

Toru Shiozaki, (Northwestern University)
"Magnetic Properties of Heavy-Element Complexes from Multireference Electron Correlation Methods"

PHEASANT ROOM 3 **Mixed III** **Chair: I. Burghardt**
David Yarkony, (Johns Hopkins University)
"Accurate Nonadiabatic Dynamics"

Trygve Helgaker, (University of Oslo)
"The Role of the Hohenberg–Kohn Theorem in Density-Functional Theory"

9:30am-10:00am **Coffee Break** 

10:00am-11:00am **Plenary VI** **Chair: T. Seideman**
BALLROOM 5
William Miller, (University of California-Berkeley)
"Symmetrical Quasi-Classical Model for Classical Molecular Dynamics Simulations of Electronically Non-Adiabatic Processes"

11:00am-12:30pm **MORNING SESSION B**
BALLROOM 5 **Per-Olov Löwdin IB** **Chair: M. Quack**
Carlos Bunge, (UNAM)
"Specifics on the Scientific Legacy of Per-Olov Löwdin"

Lawrence Dunne, (London South Bank University)

"*High Temperature Superconductivity, Long-Range Order and Broken Symmetries in Strongly Correlated Electronic Systems"*

Hazel Cox, (University of Sussex)
"Correlated Motion in Atomic and Molecular Three Particle Systems"

ORIOLE ROOM 2 **Emerging Methods IB** **Chair: F. Furche**

Alex Thom, (University of Cambridge)
"Developments in Stochastic Coupled Cluster Theory"

Lucas Wagner, (University of Illinois at Urbana-Champaign)
"Using Quantum Monte Carlo to Study Strongly Correlated Bulk Materials from First Principles"

Daniel Neuhauser, (University of California-Los Angeles)

PHEASANT ROOM 3 **Electronic Structure IVA** **Chair: Á. Szabados**

Martin Head-Gordon, (University of California-Berkeley)
"Survival of the Most Transferable: New Semi-empirical Density Functionals from a Combinatorial Design Strategy"

Wenjian Liu, (Peking University)
"New Scenarios for Strongly Correlated Electrons"

Rodney Bartlett, (University of Florida)
"The Power of Exact Conditions in Coupled-Cluster Theory and DFT"

12:30-2:00pm **ISTCP BUSINESS MEETING and LUNCH**
BLUEBIRD/FINCH ROOMS 6 & 7 **Board Members and National Representatives**

2:00pm-3:30pm **AFTERNOON SESSION A**
PHEASANT ROOM 3 **Relativistic IA** **Chair: W. Liu**

Peter Schwerdtfeger, (Massey University)
"Semi-Local All-Electron Effective Potentials for Quantum Electrodynamic Effects in 4- and 2-Component Relativistic Theories"

Gustavo Aucar, (Natural and Exact Science Faculty UNNE and IMIT CONICET Argentina)
"QED and Electron Correlation Effects, and Dia- and Paramagnetic Terms in NMR Spectroscopic Parameters"

Trond Saue, (CNRS-Université Toulouse III)
"Analytic Gradient at the 4-Component Relativistic Coupled Cluster Level with Inclusion of Spin-Orbit Coupling"

ORIOLE ROOM 2 **Emerging Methods II** **Chair: S. Hirata**

Piotr Piecuch, (Michigan University)
"Single-Reference Coupled-Cluster and Equation-of-Motion Coupled-Cluster Methods for Multi-Reference Problems: CC(P;Q) Formalism"

Marcus Reiher, (ETH Zürich)
"New Developments for the Quantum Chemical Density Matrix Renormalization Group"

Andreas Grüneis, (Max-Planck-Institute for Solid State Research)
"Towards Efficient Coupled Cluster Theories for Solids"

HAWK ROOM 5 **Chemical Insights IIA** **Chair: C. Foroutan-Nejad**

Judy I-Chia Wu, (University of Houston)
"How Do Enzymes Turn "Weak Acids" into Strong Proton Donors?"

Samantha Jenkins, (Hunan Normal University)

"Advances in QTAIM and the Stress Tensor Theory"

Shubin Liu, (University of North Carolina)
"Density Functional Reactivity Theory: Its Recent Developments and Applications"

3:30pm-4:00pm **Coffee Break** 

4:00pm-6:00pm **AFTERNOON SESSION B**

PHEASANT ROOM 3 **Relativistic IB** **Chair: P. Schwerdtfeger**

Christoph van Wüllen, (TU Kaiserslautern)
"Broken Symmetry Approach for Magnetic Properties of Oligonuclear Transition Metal Complexes"

Robert Berger, (Philipps-Universitaet Marburg)
"Relativity and Parity Violation in Molecular Systems"

Hélène Bolvin, (CNRS-Université Toulouse III)
"Magnetic properties of UO_2^+ and NpO_2^{2+}"

ORIOLE ROOM 2 **Electronic Structure IVB** **Chair: M. Musiał**

Edward Valeev, (Virginia Tech)
"Recent Advances in Reduced-Scaling Explicitly Correlated Coupled-Cluster Methods"

Dominika Zgid, (University of Michigan)
"Rigorous Quantum Embedding Using Green's Functions"

Shmuel Zilberg, (Ariel University)
"Finding Structural Principles for Strong Hydrogen Bonds"

HAWK ROOM 5 **Chemical Insights IIB** **Chair: S. Liu**

Frank Weinhold, (University of Wisconsin)
"How Hydrogen Bonding Outmuscles Electrostatics"

Eduard Matito, (Donostia Inter. Physics Center)
"Bonding Description of the Harpoon Mechanism"

Cina Foroutan-Nejad, (Masaryk University)
"Origin of Aromatic Stabilization Energy; A Route Towards Unification of Ground-State Aromaticity"

7:00pm-9:30pm **BANQUET**
BALLROOM 5

THURSDAY, JULY 21

8:00am-9:30am **MORNING SESSION A**

BALLROOM 5 **Per-Olov Löwdin IIA** **Chair: W. Miller**

Sylvio Canuto, (University Sao Paulo)
"Quantum Chemistry with Thermodynamic Condition"

Ksenia Bravaya, (Boston University)
"Electronic Structure of Metastable States with Correlated Wave Function Based Methods"

Klaus Ruedenberg, (Iowa State University)
"Quantitative Energy Decomposition Analysis of Molecular Electronic Wave Functions in Terms of Physical Contributions"

ORIOLE ROOM 2 **Relativistic IIA** **Chair: T. Saue**

Jürgen Gauss, (Universität Mainz)

"Spin-Free Relativistic Quantum Chemistry"

Lan Cheng, (Johns Hopkins University)
"Spin-Free Exact Two-Component Theory for Molecular Properties: Local Approximation for the Block Diagonalization"

Zhendong Li, (Princeton University)
"Combining Spin-Adapted Time-Dependent Density Functional Theory with Exact Two-Component Hamiltonians for Open-Shell Systems"

PHEASANT ROOM 3 **Dynamics IA** **Chair: G. Schatz**

Richard Dawes, (Missouri S&T)
"*Calculations of Spectroscopy and Scattering Dynamics using Interpolated Ab Initio Potentials"*

Bill Hase, (Texas Tech University)
"Direct Dynamics Simulations of Atomistic Mechanisms for Gas-Phase S_N2 Reactions. Comparison with Experiment and Consideration of Theoretical Method"

9:30am-10:00am **Coffee Break** 

10:00am-11:00am **Plenary VII** **Chair: J. Gauss**
BALLROOM 5
Tamar Seideman, (Northwestern University)
"Coherent Alignment in Complex Systems"

11:00am-12:30pm **MORNING SESSION B**
BALLROOM 5 **Per-Olov Löwdin IIB** **Chair: F. Weinhold**

Marco Nascimento, (Federal University of Rio de Janeiro)
"The Consequences of Neglecting Permutation Symmetry in the Description of Many-Electron Systems"

Thomas Jagau, (University of Munich)
"Non-Hermitian Quantum Mechanics in Electronic-Structure Theory"

Arik Landau, (Technion Israel)
"Resonance Complex Energies from Standard Electronic-Structure Packages via Analytic Continuation (Padé)"

ORIOLE ROOM 2 **Relativistic IIB** **Chair: R. Berger**

Stephan Sauer, (University of Copenhagen)
"On the Performance of ZORA in Calculations of NMR, EPR and PAC Parameters"

Yunlong Xiao, (Peking University)
"Relativistic Methods for NMR Shielding"

Hans Jørgen A. Jensen, (University of Southern Denmark)
"Advances in 4-Component EPR Calculations Using Configuration Interaction"

PHEASANT ROOM 3 **Dynamics IB** **Chair: ~~K. Han~~**

Geert-Jan Kroes, (Leiden University)
"Chemically Accurate Simulation of a Polyatomic Molecule-Metal Surface Reaction: Dissociative Chemisorption of CHD3 on Ni(111)"

George Schatz, (Northwestern University)
"Theory of Surface Enhanced Femtosecond Stimulated Raman Scattering"

Bret Jackson, (UMass Amherst)
"Dissociative Chemisorption Dynamics of Methane on Pt and Ni Surfaces: Mode-Specificity and Bond-Selectivity"

HAWK ROOM 5

Mixed IV **Chair: D. Zgid**

Sonia Coriani, (Aarhus University)
"Coupled Cluster Studies of Photoionization, Photodetachment and X-ray Photoabsorption"

Henrik Koch, (NTNU)
"Coupled Cluster Methods for Transient NEXAFS Spectroscopy: The Ultrafast ππ-nπ* Transition in Thymine"*

Peter Pulay, (University of Arkansas)
"Analytical Free Energy Gradients for Ultrafast Multiple Environment-Single System QM/MM Simulations"

2:00pm-3:30pm **AFTERNOON SESSION A**

BALLROOM 5

Accurate Thermochemistry IA **Chair: A. Wilson**

Branko Ruscic, (Argonne National Laboratory)
"Accurate Thermochemistry: the Why, the Rules and Conventions in Thermochemistry, and the Role of Atct as an Interface Between Theory and Experiment"

Jan Martin, (Weizmann Institute of Science)
"Toward a W4-F12 Approach: Can Explicitly Correlated and Orbital-Based Ab Initio CCSD(T) Limits be Reconciled?"

John Stanton, (University of Texas)
"The Ionization Energy of H_2O_2"

ORIOLE ROOM 2

Relativistic IIIA **Chair: Ch. van Wüllen**

Luuk Visscher, (Vrije Universiteit Amsterdam)
"Laplace-Transformed Atomic Orbital-Based Møller–Plesset Perturbation Theory for Relativistic Two-Component Hamiltonians"

Stefan Knecht, (ETH Zürich)
"The Electron Correlation Problem in the Lower Part of the Periodic Table"

PHEASANT ROOM 3

Dynamics IIA **Chair: G. Schatz**

Nandini Ananth, (Cornell University)
"Path Integral Methods for Nonadiabatic Dynamics: Quantum Transitions from Classical Trajectories"

Spriodoula Matsika, (Temple University)
"QM/MM Studies of Photoinitiated Processes in Complex Systems"

Jian Liu, (Peking University)
"Path Integral Liouville Dynamics for Quantum Correlation Functions"

3:30pm-4:00pm **Coffee Break**

4:00pm-5:00pm **Plenary VIII** **Chair: H. Bolvin**

BALLROOM 5

Martin Quack, (ETH Zürich)
"The Quantum Dynamics of Chiral and Achiral Molecules including Electroweak Parity Violation: Theory and Experiment"

5:00pm-6:30pm **AFTERNOON SESSION B**

BALLROOM 5

Accurate Thermochemistry IB **Chair: L. Curtiss**

Attila Csaszar, (ELTE)
"High-Accuracy High-Temperature Thermochemical Functions"

Wesley Allen, (University of Georgia)
"Applications of a Homodesmotic Hierarchy to High-Accuracy Thermochemistry"

Kirk Peterson, (Washington State University)
"Accurate Ab Initio Thermochemistry for Heavy Elements. Recent Results for Lanthanide- and Actinide-Containing Molecules"

ORIOLE ROOM 2 **Relativistic IIIB** **Chair: B. de Jong**

Jun Li, (Tsinghua University)

Paul Bagus, (University of North Texas)
"Inferring Chemical Properties from the Core-Level Spectra of Heavy Metal Compounds"

PHEASANT ROOM 3 **Dynamics IIB** **Chair: G. Schatz**

Artur Izmaylov, (University of Toronto)
"Geometric Phase Effects in Nonadiabatic Dynamics"

Rebecca Gieseking, (Northwestern University)
"Semiempirical Modeling of Plasmon-Enhanced Electron Transfer Processes"

FRIDAY, JULY 22

8:00am-9:30am **MORNING SESSION A**

BALLROOM 5 **Accurate Thermochemistry IIA** **Chair: A. Csaszar**

Angela Wilson, (Michigan State University)
"Advances in the Correlation Consistent Composite Approach (Ccca) Towards the Transition Metals and Heavy Elements"

Larry Curtiss, (Argonne National Laboratory)
"Application of Gaussian-4 Theory for Accurate Energies in Li-O and Li-S Systems"

Yibo Lei, (Northwest University)
"New Implementation of Static-Dynamic-Static Based Multi-Reference Perturbation Theory"

ORIOLE ROOM 2 **Emerging Methods IIIA** **Chair: R. Shepard**

Edgar Solomonik, (ETH Zürich)
"*Developing Scalable and Portable Electronic Structure Methods with Cyclops Tensor Framework"*

Robert Harrison, (Stony Brook University)
"Advances in Multiresolution and Separable Representations"

PHEASANT ROOM 3 **Relativistic IV** **Chair: J. Li**

Bert de Jong, (Lawrence Berkeley National Laboratory)
"Understanding the Role of Oxidation States on the Chemistry of Actinides"

Ephraim Eliav, (Tel Aviv University)
"Highly Accurate Heavy Atoms Calculations: From High-Precision Spectroscopy to Tests of Fundamental Physics"

9:30am-10:00am **Coffee Break**

10:00am-11:00am **Plenary IX** **Chair: S. Jenkins**

BALLROOM 5 **Ria Broer**, (University of Groningen)
"Theoretical and Computational Studies for the Design of Organic Photovoltaic Materials"

11:00am-12:30pm **MORNING SESSION B**

BALLROOM 5 **Accurate Thermochemistry IIB** **Chair: B. Ruscic**

George Schoendorff, (Michigan State University)
"Determination of Thermodynamic Properties and Spectroscopic Constants of Transition Metal and Lanthanide Containing Molecules"

David Bross, (Argonne National Laboratory)
"Active Thermochemical Tables: Uncertainties, Variances, Covariances, and Provenances"

ORIOLE ROOM 2 **Emerging Methods IIIB** **Chair: S. Ten-no**

George Booth, (King's College London)

So Hirata, (University of Illinois at Urbana-Champaign)
"Brueckner–Goldstone Quantum Monte Carlo"

David Tew, (University of Bristol)
"Explicitly Correlated Pair Natural Orbital Coupled Cluster Theory"

12:30pm-1:00pm **Closing Remarks**
BALLROOM 5