Sunday, September 14th 2014

14:00 - 17:00 Registration

17:00 - 17:10 Welcome Address

Session I Chair: Bernd M. Rode

17:10 - 17:50 **I1** Michael A. Robb
Coupled Electron-Nuclear Dynamics, using the Ehrenfest Approach

17:50 - 18:30 **I2** Eberhard K. U. Gross
How to Make the Born-Oppenheimer Approximation Exact: A Fresh Look at Potential Energy Surfaces and Berry Phases in the Vicinity of Strong Non-Adiabatic Couplings

18:30 - 19:10 **H1** Wilfried Meyer
Advances in the Methodology of Quantum Chemistry during 50 Years of the Symposium of Theoretical Chemistry

19:10 - 20:30 **Welcome Reception**

20:30 - Poster Session I

Monday, September 15th 2014

Session II Chair: Peter W. Langhoff

9:00 - 9:40 **I3** Andreas Dreuw
The Algebraic Diagrammatic Construction for the Polarization Propagator - a Versatile Approach to Excited Electronic States, Ionization Potentials and Electron Affinities

9:40 - 10:00 **C1** Monika Srebro
Delocalization Error and "Functional Tuning" in Kohn-Sham Calculations of Molecular Properties

10:00 - 10:20 **C2** Christoph Bannwarth
The Simplified TD-DFT and TDA Approaches: Excited States and Spectra for Very Large Systems

10:20 - 10:50 **Coffee Break**

Session III Chair: Christoph van Wüllen

10:50 - 11:30 **I4** Garnet Kin-Lic Chan
Quantum Chemistry in the Condensed Phase

11:30 - 11:50 **C3** Peter Schwerdtfeger
Toward an Accurate Description of Rare Gas Phases

11:50 - 12:10 **C4** Stefan Knecht
Relativistic Density Matrix Renormalization Group

12:10 - 12:30 **C5** Örs Legeza
Generalized Tensor Methods and Entanglement Measurements for Electronic Structure Calculations

12:30 - 14:00 **Lunch**

Session IV Chair: Willem Klopper

14:00 - 14:40 **I5** Hans-Joachim Werner
Scalable Electron Correlation Methods

14:40 - 15:20 **I6** Roland Lindh
Cholesky Photo Chemistry: Theory, Implementation and Performance

15:20 - 15:40 **C6** Pedro B. Coto
The Low-Lying Electronic Excited States of Pentacene Oligomers: An Electronic Structure Study in the Context of Singlet Fission

15:40 - 16:00 **C7** Florian A. Bischoff
Regularizing Singularities in the Molecular Potential

16:00 - 16:30 **Coffee Break**

Session V Chair: Leticia González

16:30 - 17:10 **E1** Nuno Maulide
Chemistry Meets Piano: 3000 Years of Music

Session VI Chair: W. H. Eugen Schwarz

17:10 - 18:45 **H2** Klaus Ruedenberg
Three Millennia of Atoms, Molecules and Bonds

18:45 - 19:45 **Dinner**

19:45 - Poster Session II

Tuesday, September 16th 2014

Session VII Chair: Horst Köppel

9:00 - 9:40 **I7** Walter Thiel
Surface-Hopping Excited-State Dynamics

9:40 - 10:00 **C8** Iakov Polyak
Quantum Dynamics on-the-fly: Development and Applications of the Direct Dynamics Variational Multiconfigurational Gaussian Method

10:00 - 10:20 **C9** Sebastian Thallmair
Reactive Molecular Wave Packet Dynamics Directed by Explicit Solvent Cage

10:20 - 10:50 **Coffee Break**

Session VIII Chair: Paul Popelier

10:50 - 11:30 **I8** Marcus Elstner
Mixed Quantum-Classical Fragment Orbital based Non-Adiabatic Molecular Dynamics Simulations for Charge Transfer in Complex Systems

11:30 - 11:50 **C10** Bettina G. Keller
Variational Approach to Molecular Dynamics

11:50 - 12:10 **C11** Lars Schäfer
Fully Flexible Protein-Protein Docking: Predicting Protein Complexes from All-Atom MD Simulations

12:10 - 12:30 **C12** Matthias Heyden
Spatial Resolution of Long-Ranged Dynamical Coupling between Proteins and Hydration Water

12:30 - 14:00 **Lunch**

Session IX Chair: Philipp Marquetand

14:00 - 14:40 **I9** Benedetta Mennucci
Structural and Environmental Effects in Natural Light-Harvesting Antennae: A Quantum Chemical Analysis

14:40 - 15:00 **C13** Mark P. Waller
A Density-Based Adaptive QM/MM Method

15:00 - 15:20 **C14** Antonio Monari
Excited States in Biological Relevant Systems: DNA Photosensitization

15:20 - 15:40 **C15** Keyarash Sadeghian
QM/MM Study on Ribose-Protonated DNA Base-Excision Repair

15:40 - 16:00 **C16** Artur Nenov
Tracking Conformational Dynamics of Peptides by Nonlinear Electronic Spectroscopy of Aromatic Residues: Ab-initio Simulations Beyond the Frenkel Exciton Hamiltonian

16:00 - 16:30 **Coffee Break**

Session X Chair: Alexander Sax

16:30 - 17:10 **I10** Angela K. Wilson
Electronic Structure and Energetics Towards Quantitative Accuracy: Dynamic and Non-Dynamic Electron Correlation from the Main Group to the Heaviest Elements

17:10 - 17:50 **I11** Jürgen Gauss
Quantum Chemistry Meets Rotational Spectroscopy: The Quest for High Accuracy

17:50 - 18:45 Lecture Hall C1 - Bob van Daalen (Elsevier)
Author Workshop - How to Sucessfully Publish Scientific Articles

Lecture Hall C2 - Business meeting of the AGTC (*Arbeitsgemeinschaft Theoretische Chemie*)

18:45 - 19:45 **Dinner**

19:45 - Poster Session III

Wednesday, September 17th 2014

Session XI Chair: Christian Ochsenfeld

9:00 - 9:40 *Hellmann Award Lecture*

9:40 - 10:00 **C17** Sergey I. Bokarev
Theoretical Soft X-Ray Spectroscopy of Transition Metal Compounds in Solution

10:00 - 10:20 **C18** Thomas Renger
The Role of Electrostatics and Quantum Dynamics in the Modeling of Optical Spectra and Energy Transfer in Chromophore-Protein Complexes

10:20 - 10:50 **Coffee Break**

Session XII Chair: Beate Paulus

10:50 - 11:30 **I12** Irene Burghardt
Quantum Dynamics of Exciton Migration and Dissociation in Functional Organic Polymer Materials

11:30 - 11:50 **C19** Jean Christophe Tremblay
Manipulating Subsurface Hydrides in Palladium via Scanning Tunnelling Microscopy

11:50 - 12:10 **C20** Judith B. Rommel
Chemisorption on Metal Surfaces: The Role of Quantum Tunnelling

12:10 - 12:30 **C21** M. Verónica Ganduglia-Pirovano
The Role of Electron Localization in the Catalytic Function of Cerium-Oxide-based Systems

12:30 - 14:00 **Lunch**

14:00 - 18:00 *Excursions/Free Afternoon*

19:00 - 22:45 *Conference Dinner*

Thursday, September 18th 2014

Session XIII Chair: Regina de Vivie-Riedle

9:00 - 9:40 **I13** Peter Saalfrank
Dynamics in Molecules after Photoinduced Electronic Excitations

9:40 - 10:00 **C22** Jesús González-Vázquez
Strong Field Control of Ultrafast Photodissociation: A Molecular Example of Dynamics through Light-Induced Conical Intersections

10:00 - 10:20 **C23** Monika Leibscher
Selective Control of Rotational Dynamics: Applications to Nuclear Spin Isomers and Enantiomers

10:20 - 10:50 **Coffee Break**

Session XIV Chair: Jörn Manz

10:50 - 11:30 **I14** Ivano Tavernelli
Nonadiabatic Dynamics of Complex Molecular Systems based on Time-Dependent Density Functional Theory

11:30 - 11:50 **C24** Carmen Herrmann
Comparative Studies of Electronic Communication through Molecular Bridges

11:50 - 12:30 **I15** Todd J. Martínez
Leveraging Machine Learning and Stream Processors to Simulate and Discover Chemical Reactions

12:30 - 13:00 *Closing / Poster Prizes*