Tuesday, September 8, 2009

15:00 Registration, Coffee

17:30 Christel M. Marian, Düsseldorf
Opening

Session 1 Chair: Bernd Engels

17:40 **I-1** Sigrid Peyerimhoff, Bonn
The study of electronic spectra of molecules in the early days of digital computing

18:20 **I-2** Sam Leutwyler, Bern
π-Stacking in gas-phase dimers: A spectroscopic perspective

19:00 Welcome Reception

19:30 Dinner

Wednesday, September 9, 2009
Morning Sessions

Session 2 Chair: Walter Thiel

9:00 I-3 Jun-ya Hasegawa, Kyoto
Excited states of photofunctional molecules in protein: Electronic structure and interaction

9:40 C-1 Petra Imhof, Heidelberg
Exploring the green-to-red conversion in the fluorescent protein EOSFP

10:00 C-2 Lars Goerigk, Münster
Application of time-dependent double-hybrid density functional theory to electronic excited states

10:20 C-3 Marius Wanko, San Sebastian
Advances in QM/MM modeling of protein spectroscopy

10:40 Coffee break

Session 3 Chair: Hans Lischka

11:10 I-4 Peter Gilch, Düsseldorf
The photochemistry of o-nitrobenzaldhyde - challenges for the theoretician and the experimentalist

11:50 C-4 Tatiana Domratcheva, Heidelberg
A non-oxetane DNA photorepair pathway: Electronic structure of the (6-4) photoproduct radical anion and its repair reaction

12:10 C-5 Tomáš Kubař, Braunschweig
Time-dependent DFT simulation of charge transfer in DNA

12:30 C-6 Oliver Kühn, Rostock
Two-dimensional infrared spectroscopy of the correlated dynamics of the adenine:uracil hydrogen bonds in solution

13:00 Lunch

Wednesday, September 9, 2009
Afternoon Sessions

Session 4 Chair: Dominik Marx

15:00 **I-5** Jörn Manz, Berlin
Quantum control by laser pulses: From nuclear to electron dynamics, and back

15:40 **C-7** Anthony Dutoi, Heidelberg
Tracing ultrafast molecular electronic energy transfer in real time and space

16:00 **C-8** Anna Stradomska, Groningen
Exciton-phonon coupling in self-assembled porphyrin nanotubes

16:20 **C-9** Susanta Mahapatra, Hyderabad
Quantum dynamics of electronically excited molecules

16:40 Coffee break

Session 5 Chair: Wolfgang Domcke

17:10 **I-6** Andrzej L. Sobolewski, Warsaw
Photophysics of hydrogen bonds: From theory to applications

17:50 **C-10** Lluís Blancafort, Girona
Photodynamics of thymine: potential energy surface and quasi-classical dynamics

18:10 **C-11** Artur Nenov, München
The conical intersection seam for fulgides and the influence of substituent effects on the photoreaction

18:30 **C-12** Peter Deglmann, Ludwigshafen
Accurate prediction of radical propagation rate cofficients

19:00 Dinner

20:00 Posters, odd numbers

Thursday, September 10, 2009

Session 6 Chair: Stefan Grimme

9:00 **I-7** William Lester Jr., Berkeley
Quantum Monte Carlo for the electronic structure of molecules

9:40 **C-13** Jörg Behler, Bochum
Neural network potential-energy surfaces: from elemental solids to multicomponent systems

10:00 **C-14** Michael Springborg, Saarbrücken
From dipole moment to polarization - the missing link

10:20 **C-15** K.D. Sen, Hyderabad
Importance of second derivative of electron density at origin

10:40 Coffee break

Session 7 Chair: Martin Schütz

11:10 **I-8** Ove Christiansen, Århus
One- and two-photon absorption of molecules in gas and liquid phase

11:50 **C-16** Andreas Köhn, Mainz
Challenges in explicitly correlated coupled-cluster theory: excited states and connected higher-order clusters

12:10 **C-17** Lasse K. Sørensen, Düsseldorf
Implementation and initial application of a general-order 4-component multi-reference coupled-cluster program

12:30 **C-18** Alexander A. Auer, Chemitz
Efficiency and controllable error in a screening-based coupled cluster approximation

13:00 Lunch

15:00 Excursion

19:00 Conference Dinner

Friday, September 11, 2009
Morning Sessions

Session 8 Chair: Bernd Hartke

9:00 I-9 Michael A. Robb, London
Quadratic description of conical intersections: Applications to structure, spectroscopy and dynamics

9:40 C-19 Matthias Ruckenbauer, Wien
Hybrid multiple-method for MRCI gradients and their application to nonadiabatic dynamics

10:00 C-20 Johannes Kästner, Stuttgart
How to find transition states inC many thousand degrees of freedom? The dimer method improved for QM/MM simulations of enzymes

10:20 I-21 Oliver Weingart, Essen
Mechanistic and spectroscopic features in the rhodopsin primary event from theory and experiment

10:40 Coffee break

Session 9 Chair: Peter Saalfrank

11:10 I-10 Irene Burghardt, Paris
Ultrafast photophysics of organic semiconductor junctions: a molecular-level, quantum-dynamical perspective

11:50 C-22 Sibylle Gemming, Chemnitz
Novel concepts for anisotropic Heisenberg modeling of multiferroic oxides

12:10 C-23 Itai Panas, Göteborg
Origin and properties of checkerboard electronic structure in the cuprates of possible relevance to high T_c superconductivity

12:30 C-24 Jean Christophe Tremblay, Potsdam-Golm
Electronic damping of adsorbate vibrations at metallic surfaces

13:00 Lunch

Friday, September 11, 2009
Afternoon Sessions

Session 10 Chair: Gernot Frenking

15:00 **I-11** Christian Lennartz, Ludwigshafen
Photopysics and charge transport properties of OLED-materials

15:40 **C-25** Denis Usvyat, Regensburg
Periodic local MP2 and CIS models with density fitting

16:00 **C-26** Oscar Rubio Pons, Erlangen
Theoretical analysis of excited states in chromophore-titanium oxide complexes: A benchmark study

16:20 **C-27** Christoph van Wüllen, Kaiserslautern
On the DFT calculation of magnetic anisotropies for multinuclear complexes

16:40 Coffee break

Session 11 Chair: Gernot Frenking

17:10 **I-12** Anne-Marie Kelterer, Graz
Quantum chemical modeling of excited state properties of sensing-active materials and phosphorescent Eu-complexes

17:50 **DFG** Johanna Kowol-Santen, DFG
Neues bei der Deutschen Forschungsgemeinschaft

18:10 AGTC Vollversammlung

19:00 Dinner

20:00 Posters, even numbers

Saturday, September 12, 2009

Session 12 Chair: Uwe Manthe

9:00 **I-13** Todd Martinez, Stanford
Photochemistry and mechanochemistry from first principles dynamics

9:40 **C-28** Milan Ončák, Prague
Photochemistry of atmospherically relevant species(CH_2O, H_2O_2, NO_3^-) in the gas phase, in water droplets and on ice

10:00 **C-29** Jörg Tatchen, Düsseldorf
On-the-fly computation of vibronic spectra for strongly anharmonic systems

10:20 **C-30** Zhenggang Lan, Mülheim
Excited-state dynamics: on-the-fly surface-hopping studies with the semiempirical OM2 method

10:40 Coffee break

Session 13 Chair: Arne Lüchow

11:10 **I-14** Nikos L. Doltsinis, London
Multiscale modelling of photoactive materials

11:50 **C-31** Daniel Sebastiani, Mainz
Hydrogen bond dynamics in proton conductors from ab-initio molecular dynamics simulations and spectroscopy

12:10 **C-32** Sergei Ivanov, Bochum
Quantum-induced symmetry breaking explains infrared spectra of CH_5^+ isotopologues

12:30 Andreas Dreuw, Frankfurt
Closing

13:00 Lunch, Departure