Programme

Sunday, September 16th

Reception

17.00 – 20.00 Registration in the Town Hall of the Town of Saarbrücken

18.00 – 20.00 Reception in the Town Hall of the Town of Saarbrücken

Monday, September 17th

From 7.45 Registration in front of the lecture hall

Session 1

Chair: Gernot Frenking (Marburg, Germany)

8.30 – 8.35 Michael Springborg (Saarbrücken, Germany): *Opening*

8.35 – 9.20 I1: Dominik Marx (Bochum, Germany): *Recent trends in ab initio simulation*

9.20 – 9.40 C1: Daniel Sebastiani (Mainz, Germany): *Proton momentum-space densities from first-principles path-integral molecular dynamics simulations*

9.40 – 10.00 C2: Petr Slavicek (Prague, Czech Republic): *Photochemical reactions studied by ab initio quantum molecular dynamics: from molecules to clusters*

10.00 – 10.30 Break

Session 2

Chair: Christoph van Wüllen (Berlin, Germany)

10.30 – 11.15 I2: Richard L. Martin (Los Alamos, USA): *The localization / delocalization dilemma in the electronic structure of f-element oxides*

11.15 – 11.35 C3: Anatoly Titov (St. Petersburg, Russia): *Combined ab initio methods and accurate study of heavy-atom molecules to search for new physics beyond the standard model*

11.35 – 11.55 C4: Hélène Bolvin (Strasbourg, France): *Calculation of electronic g-matrices of actinide compounds*

11.55 – 13.30 Lunch break

Session 3

Chair: W. H. Eugen Schwarz (Siegen, Germany)

13.30 – 14.15 I3: John P. Perdew (New Orleans, USA): *Hyper-generalized gradient approximation for the exchange-correlation energy of density functional theory*

14.15 – 14.35 C5: Katrick Gupta (Bordwan, India): *A DFT study of acidity of ortho- and para-substituted aromatic acids using molecular descriptors*

14.35 – 14.55 C6: Laszlo von Szentpaly (Stuttgart, Germany): *Critique and correction of conceptal DFT*

14.55 – 15.30 Break

Session 4

Chair: Christel Marian (Düsseldorf, Germany)

15.30 – 16.15 I4: Poul Jørgensen (Århus, Denmark): *A ground-state directed optimization scheme for the Kohn-Sham energy*

16.15 – 16.35 C7: Christian Ochsenfeld (Tübingen, Germany): *A linear-scaling AO-based MP2 method for large molecules by rigorous integral estimates*

16.35 – 16.55 C8: Andreas Köhn (Mainz, Germany): *Excitation energy transfer rates from correlated transition densities*

16.55 – 17.45 Break

Session 5

Chair: Thomas Heine (Dresden, Germany)

17.45 – 18.30 I5: Benoît Champagne (Namur, Belgium): *Ab initio polymer quantum theory: structural and vibrational properties*

18.30 – 19.30 Dinner

Poster session 1

19.30 – 22.00 Posters with odd numbers. (Including free beverages)

Tuesday, September 18th

From 8.35 Registration in front of the lecture hall

Session 6

Chair: Wolfgang Domcke (Munich, Germany)

8.35 – 9.20 Presentation of the Hellmann Prize winner

9.20 – 9.40 C9: Serguei Fomine (Mexico City, Mexico): *Tubular aggregates of cyclic oligothiophenes. A theoretical study*

9.40 – 10.00 C10: Alisa Krishtal (Antwerp, Belgium): *The effect of structural parameters on the polarizabilities of methanol clusters: a Hirshfeld study*

10.00 – 10.30 Break

Session 7

Chair: Gotthard Seifert (Dresden, Germany)

10.30 – 11.15 I6: Benedetta Mennucci (Pisa, Italy): *Structure and properties of molecular solutes in electronic excited states: a quantum mechanical Polaizable Continuum Model*

11.15 – 11.35 C11: Jan-Ole Joswig (Dresden, Germany): *Proton transport in liquid phosphonic acid and polyphosphonic acid based polymers studied with molecular-dynamics simulations*

11.35 – 11.55 C12: Tillmann Klamroth (Potsdam, Germany): *Explicitly time-dependent configuration interaction simulations: dipole switching in large molecules*

11.55 – 13.30 Lunch break

Session 8

Chair: Georg Jansen (Essen, Germany)

13.30 – 14.15 I7: Joachim Sauer (Berlin, Germany): *Structure and reactivity of oxide catalysts*

14.15 – 14.35 C13: Judith Voll (Munich, Germany): *Laser induced femtosecond dynamics in the excited states of beta-carotene*

14.35 – 14.55 C14: Ozlem Ozcan (Düsseldorf, Germany): *A Monte Carlo – DFT study: adsorption of organosilanes on polar ZnO(0001) surfaces*

14.55 – 15.30 Break

Session 9

Chair: Dirk Andrae (Bielefeld, Germany)

15.30 – 16.15 I8: Arne Lüchow (Aachen, Germany): *Electron structure quantum Monte Carlo: recent developments and applications*

16.15 – 16.35 C15: Vincent Tognetti (Paris, France): *DFT study of ethylene dimerization by mixed bidentate P–N nickel complexes*

16.35 – 16.55 C16: Philipp Scherer (Munich, Germany): *Nonadiabatic coupling mechanism for ultrafast electron transfer in the reaction center of bacterial photosynthesis*

17.30 – 18.15 Break

Session X

Chair: Wolfgang Domcke (Munich, Germany)

17.30 – 18.00 X: Frank-Dieter Kuchta (DFG, Germany): *Die Deutsche Forschungsgemeinschaft informiert!*

18.00 – 18.30 Mitgliederversammlung AGTC

Poster session 2

19.30 – 22.00 Posters with even numbers. (Including free beverages)

Wednesday, September 19th

From 8.35 Registration in front of the lecture hall

Session 10

Chair: Daniel Sebastiani (Mainz, Germany)

8.35 – 9.20 I9: Karlheinz Schwarz (Vienna, Austria): *DFT calculations of crystals and surfaces with WIEN2k*

9.20 – 9.40 C17: David Benoit (Ulm, Germany): *Accurate computation of vibrational spectra for extended systems*

9.40 – 10.00 C18: Liviu Hozoi (Dresden, Germany): *Correlated bands in oxides with wave-function based methods*

10.00 – 10.30 Break

Session 11

Chair: Beate Paulus (Dresden, Germany)

10.30 – 11.15 I10: David Wales (Cambridge, UK): *Energy landscapes: from clusters to biomolecules*

11.15 – 11.35 C19: Konstantin Neyman (Barcelona, Spain): *Nanosized metal and oxide particles as realistic models of catalytic materials*

11.35 – 11.55 C20: Christoph Scheurer (Mainz, Germany): *Simulation of photoluminescence spectra of neutral and charged exciton states in self-assembled semiconductor quantum dot molecules*

12.00 – 19.30 Excursion

19.30 – ? Conference Dinner

Thursday, September 20th

From 8.35 Registration in front of the lecture hall

Session 12

Chair: Frank Neese (Bonn, Germany)

8.35 – 9.20 I11: Martin Kaupp (Würzburg, Germany): *Magnetic properties and local hybrid functionals*

9.20 – 9.40 C21: Dominik Kröner (Potsdam, Germany): *Laser-controlled chiral molecular switch: Quantum simulations for the stereoselective transformation between achiral and chiral atropisomers*

9.40 – 10.00 C22: Wolfgang Eisfeld (Bielefeld, Germany): *Taming of a beast: Multi-mode nonadiabatic excited state dynamics in NO_3*

10.00 – 10.30 Break

Session 13

Chair: Michael Bühl (Mühlheim, Germany)

10.30 – 11.15 I12: Hermann Stoll (Stuttgart, Germany): *Long-range correlation and local increments*

11.15 – 11.35 C23: Beate Paulus (Dresden, Germany): *Adsorption energy calculations with the method of increments: application to the adsorption of CO on the CeO_2(110) surface*

11.35 – 11.55 C24: Ulrich Wedig (Stuttgart, Germany): *Bonding properties in elemental Zn and Cd*

Closing

Chair: Michael Springborg (Saarbrücken, Germany)

11.55 Anne-Marie Kelterer (Graz, Austria): Presentation of the 44th Symposium for Theoretical Chemistry, 2008

Poster Prize Board: Presentation of the winners of the poster prizes

Closing

Lunch

Departure