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 Wülken (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)


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


14.55 – 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*

10.00 – 10.30 Break

Session 7

Chair: Gotthard Seifert (Dresden, Germany)


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


16.35 – 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 NO₃

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 CeO₂(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