

# 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: Katrik 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 conceptual 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 Polarizable 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<sub>3</sub>*

**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<sub>2</sub>(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