
Sunday, September 26, 2010

15:00 Registration and Coffee

17:00 STEFAN GRIMME, Münster

Opening

Session 1 Chair: Andreas Köhn

17:20 I-1 MARTIN SUHM, Göttingen

Probing molecular recognition benchmarks for electronic structure theory: vibrational spectroscopy in supersonic jets

18:10 C-1 ANDREAS KLAMT, Leverkusen

COSMO-RS: from quantum chemistry to fluid phase thermodynamics and mesoscale systems

18:30 C-2 ALEXANDER A. AUER, Düsseldorf

Tensor product approximation techniques in post-HF methods

18:50 Welcome Reception

Monday, September 27, 2010
Morning Sessions

Session 2 Chair: Johannes Neugebauer

09:00 I-2 ULF RYDE, Lund

Comparison of QM cluster calculations and QM/MM calculations for reactions in proteins

09:50 C-3 ŁUKASZ WALEWSKI, Bochum

Full quantum simulations of molecules in superfluid helium

10:10 C-4 THOMAS D. KÜHNE, Mainz

Second generation Car-Parrinello molecular dynamics: theory and application to the liquid/vapor interface

10:30 Coffee

Session 3 Chair: Christian Ochsenfeld

11:00 I-3 JEREMY N. HARVEY, Bristol

Organometallic and bioinorganic catalysis: computational insight into complex systems

11:50 C-5 GERHARD TAUBMANN, Ulm

Packing effects in the solid state structure of molecular crystals

12:10 C-6 A. DANIEL BOESE, Essen

DFT-SAPT based on ab initio potentials

12:30 C-7 STEPHAN N. STEINMANN, Lausanne

A system-dependent density-based dispersion correction

12:50 Break

Monday, September 27, 2010
Afternoon Sessions

Session 4 Chair: Andreas Dreuw

14:30 I-4 DAVID J. TOZER, Durham

TDDFT excited states: challenges & solutions

15:20 C-8 JOHANNES NEUGEBAUER, Leiden

Subsystem TDDFT for biomolecular spectroscopy

15:40 C-9 DOMINIK KRÖNER, Potsdam

Chiral distinction by femtosecond laser ionization

16:00 Coffee

Session 5 Chair: Beate Paulus

16:30 I-5 FILIPP FURCHE, Irvine

The hartree of correlation

17:20 C-10 ANDREAS HESSELMANN, Erlangen

Assessment of a new orbital-dependent exchange-correlation functional based on the Random Phase Approximation with exact Kohn-Sham exchange

17:40 C-11 ROBIN HAUNSCHILD, Houston

Range-separated local hybrids

18:00 C-12 DANIEL R. ROHR, Łódź

Short-range density functional theory and long-range density matrix functional theory

19:00 Poster Session I, **Posters 1-102**

Tuesday, September 28, 2010
Morning Sessions

Session 6 Chair: Max Holthausen

09:00 I-6 JAY S. SIEGEL, Zürich

Aromatic architectures: bowls, gears, and knots

09:50 C-13 JUDITH ROMMEL, Stuttgart

Tunneling rates in the enzyme glutamate mutase: the instanton method applied to large systems

10:10 C-14 JAN BOYKE SCHÖNBORN, Kiel

Ab-initio and semi-empirical molecular dynamics studies of E-iPr-furylfulgide

10:30 Coffee

Session 7 Chair: Daniel Sebastiani

11:00 I-7 DAVID J. WALES, Cambridge (UK)

Energy landscapes: from molecules to motors

11:50 C-15 JOHANNES HACHMANN, Cambridge (US)

Grid based quantum chemistry: a large-scale screening of molecular motifs for organic photovoltaics

12:10 C-16 RALF TONNER, Marburg

Adsorption of proline and glycine on the TiO₂(110) surface - a DFT study

12:30 C-17 SERGIO TOSONI, Berlin

Accurate quantum chemical energies for the interaction of hydrocarbons with oxide surfaces

12:50 Break and Excursions

19:00 Conference Dinner

Wednesday, September 29, 2010
Morning Sessions

Session 8 Chair: Dominik Marx

09:00 Hellmann-Award

09:50 C-18 REINHOLD F. FINK, Würzburg

S₂-Perturbation theory

10:10 C-19 MAREK SIERKA, Berlin

Resolution of identity approximation for the Coulomb term in molecular and periodic systems

10:30 Coffee

Session 9 Chair: Andreas Heßelmann

11:00 I-8 SO HIRATA, Urbana

First-principles electronic and vibrational methods for solids

11:50 C-20 CARSTEN MÜLLER, Berlin

Electron correlation contribution to adsorption energies

12:10 C-21 THOMAS BREDOW, Bonn

The role of dispersion effects in the adsorption of organic molecules at metal and insulator surfaces

12:30 C-22 THOMAS HEINE, Bremen

Assessing the hydrogen adsorption in covalent organic frameworks

12:50 Break

Wednesday, September 29, 2010
Afternoon Sessions

Session 10 Chair: Johannes Kästner

14:30 I-9 MARTIN SCHÜTZ, Regensburg

Local correlation methods for periodic systems

15:20 C-23 K. R. SHAMASUNDAR, Stuttgart

A new internally contracted multi-reference configuration interaction method: theory, implementation and applications

15:40 C-24 FRANCESCO A. EVANGELISTA, Mainz

Is internally contracted multireference coupled cluster theory the way to go?

16:00 Coffee

Session 11 Chair: Johannes Kästner

16:30 I-10 MICHAEL HANRATH, Köln

Recent advances in the implementation and application of general order coupled cluster methods

17:20 MIRIAM DIERKER, Alexander-von-Humboldt-Stiftung

17:40 KARL JUG, Hannover

Genealogie der Theoretischen Chemie

18:00 AGTC-Meeting

19:00 Poster Session II, **Posters 103-203**

Thursday, September 30, 2010
Morning Sessions

Session 12 Chair: Alexander Auer

09:00 I-11 JÜRGEN GAUSS, Mainz

Computational thermochemistry with chemical accuracy

09:50 C-25 WIM KLOPPER, Karlsruhe

Sub-meV accuracy in first-principles computations of atomic ionization potentials and electron affinities

10:10 C-26 Martin Korth, Cambridge (UK)

Accurate thermochemistry with fixed-node diffusion Monte Carlo

10:30 Coffee

Session 13 Chair: Marek Sierka

11:00 I-12 PETER M. W. GILL, Canberra

New insights into DFT from electrons on a sphere

11:50 C-27 JOACHIM FRIEDRICH, Köln

The incremental scheme for local electron correlation calculations

12:10 C-28 RICARDO MATA, Göttingen

Calculation of electronic excitation energies in molecules through the use of incremental correlation schemes

12:30 STEFAN GRIMME, Münster

Closing

12:50 Departure