Third Meeting of the DFG Priority Program 1145

Modern and universal first-principles methods for many-electron systems in chemistry and physics

July 4-6, 2005

CJD Bonn, Graurheindorfer Str. 149, D-53117 Bonn,
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Program (version June 28, 2005)

Monday, July 4, 2005

until 12:00	**Arrival**
12:00 - 14:00	**Lunch**
13.30 - 14:00	**Review panel board:** First meeting (with Dr. Kuchta, DFG)
	Project applicants: Please put posters on display !
	Oral presentations I
14:00 - 14:20	Welcome (Dr. Kuchta, DFG; Prof. Dr. Dolg, Cologne)
14:20 - 14:55	Hans-Joachim Werner (Stuttgart)
	Local explicit correlation methods
14:55 - 15:05	Discussion
15:05 - 15:25	Michael Hanrath (Köln)
	An exponential multi-reference wavefunction ansatz
15:25 - 15:30	Discussion
15:30 - 16:15	**Coffee break**
	Oral presentations II
16:15 - 16:50	Eberhard Gross (Berlin)
	The fundamental gap in reduced-density-matrix-functional theory
16:50 - 17:00	Discussion
17:00 - 17:20	Burkhard Fricke (Kassel)
	Non-collinear calculation of the magnetic (and electric) properties of small molecules and clusters as a function of the size
17:20 - 17:25	Discussion
17:25 - 17:45	Martin Kaupp (Würzburg)
	Development and implementation of modern density functional methods for property calculations
17:45 - 17:50	Discussion
18:00 - 19:30	**Dinner**
	Poster session I
19:30 - 22:00	Discussion of the project applicants with the members of the review panel board at the posters

Tuesday July 5, 2005

7:00 - 9:00	**Breakfast**
	Oral presentations III
9:00 - 9:35	Michael Griebel (Bonn) *A dimension-adaptive sparse grid method for the Schrödinger equation*
9:35 - 9:45	Discussion
9:45 - 10:05	Reinhold Schneider (Kiel) *Operator calculus of density matrices and sparse wavelet representations*
10:05 - 10:10	Discussion
10:10 - 10:20*	Dietmar Kolb or Hongjun Luo (Kassel) *A linearized approach to relativistic minimax (LARM) for many particle systems*
10:20 - 10:30*	Christoph van Wüllen (Berlin) *Development of an efficient and quasirelativistic two-component program package for Hartree-Fock and density functional calculations*
10:30 - 11:00	**Coffee break**
	Oral presentations IV
11:00 - 11:35	Markus Reiher (Jena) *Convergence characteristics of Quantum Chemical DMRG Calculations*
11:35 - 11:45	Discussion
11:45 - 12:05	Hermann Stoll (Stuttgart) *Coupling of density-functional and configuration-interaction type methods*
12:05 - 12:10	Discussion
12:10 - 12:20*	Georg Jansen (Essen) *Three-body intermolecular interactions with a combined density functional and symetry-adapted perturbation theory approach*
12:20 - 12:30*	Christian Ochsenfeld (Tübingen) *Development of a linear-scaling MP2 method for large molecules by rigorous integral criteria*
12:30 - 14:00	**Lunch**
	Oral presentations V
14:00 - 14:35	Manuel Richter (Dresden) *Orbital magnetism in molecules and solids*
14:35 - 14:45	Discussion
14:45 - 15:05	Stefan Kurth (Berlin) *Optimized effective potentials in current-density functional theory*
15:05 - 15:10	Discussion
15:10 - 15:20*	Helmut Eschrig (Dresden) *Test and improvement of current density functionals using an exactly solvable two-electron model*
15:20 - 15:30*	Daniel Sebastiani (Mainz) *Van-der-Waals-forces in density functional theory electronic structure calculations*
15:30 - 16:15	**Coffee break**

Oral presentations VI

16:15 - 16:50	Arno Schindlmayr (Jülich) *Electronic structure and excitation spectra of periodic solids within first-principles many-body perturbation theory*
16:50 - 17:00	Discussion
17:00 - 17:20	Martin Schütz (Regensburg) *Development of local electron corelation methods for periodic systems*
17:20 - 17:25	Discussion
17:25 - 17:35*	Beate Paulus (Dresden) *Development of a wavefunction-based ab-initio method for group II metals applying the method of increments*
17:35 - 17:45*	Alejandro Saenz (Berlin) *Ab-initio treatment of systems with translational symmetry using confined Gaussians*
17:45 - 17:55*	Michael Springborg (Saarbrücken) *Development and implementation of theoretical methods for dealing with functions of the quantum-mechanical operator r in extended systems*
18:00 - 19:30	**Dinner**
18:00 - ...	**Review panel board:** Second meeting

Oral presentations VII

19:30 - 20:05	Jürgen Gauss (Mainz) *Higher excitations in coupled cluster theory*
20:05 - 20:15	Discussion

Poster session II/SPP 1145 Meeting

20:15 - 22:00	Discussion of the project applicants with the members of the review panel board at the posters (only if required by the review panel) **or alternatively** business meeting SPP 1145 (future directions, workshops, symposium 2006, etc.)

Wednesday July 6, 2005

7:00 - 9:00	**Breakfast**
9:00 - ...	**Review panel board**: Third meeting (if required)
	Oral presentations VIII
9:00 - 9:35	Trond Saue (Strasbourg)
	Perspectives on 2- and 4-component relativistic calculations
9:35 - 9:45	Discussion
9:45 - 10:20	Claudia Filippi (Leiden)
	Quantum Monte Carlo for ground and excited-state calculations
10:20 - 10:30	Discussion
10:30 - 11:00	**Coffee break**
	Oral presentations IX
11:00 - 11:35	Andreas Savin (Paris)
	The multi-configuration Kohn-Sham method
11:35 - 11:45	Discussion
11:45 - 12:20	Stefan Goedecker (Basel)
12:20 - 12:30	Discussion
	Global minimum determination of the Born-Oppenheimer surface within density functional theory
12:30 - 14:00	**Lunch**
	Departure

* presentation of new project proposals. Note: the time of 10 minutes includes the time for discussion (e.g., 7 minutes talk plus 3 minutes discussion).