PROGRAM

Time	Monday 26.06.2006	Tuesday 27.06.2006	Wednesday 28.06.2006
09:00 - 09:50		F. Furche	G. Kresse
09:50 - 10:25		C. Hättig	U. Birkenheuer
10:25 - 10:45		S. Pittalis	T. Scott
10:45 - 11:15		Coffee	Coffee
11:15 - 12:05		F. Manby	R. J. Harrison
12:05 - 12:40	Arrival	T. Fleig	M. Dolg
13:00 - 14:30	Lunch	Lunch	Lunch
14:30 - 15:20	K. Burke	M. Head-Gordon	Departure
15:20 - 15:55	C. van Wüllen	C. Ochsenfeld	
15:55 - 16:25	Coffee	Coffee	
16:25 - 17:15	P. Pulay	M. Nooijen	
17:15 - 17:35	S. Eckard	M. Hanrath	
17:35 - 17:55	E. Kordel	M. Nest	
18:00 - 20:00	Dinner	Conf. Dinner	
20:00 - 23:00	Poster		

Monday, 26 June 2006

12:05 – 12:40	Arrival
13:00 – 14:30	Lunch
14:30 – 15:20	**K. Burke** (Rutgers University, Piscataway) *Quantum defect in time-dependent density functional theory*
15:20 – 15:55	**C. van Wüllen** (TU Berlin) *Two-component quasirelativistic computational methods*
15:55 – 16:25	Coffee
16:25 – 17:15	**P. Pulay** (University of Arkansas, Fayetteville) *Using plane waves and Gaussians in molecular quantum chemistry*
17:15 – 17:35	**S. Eckard** (Universität Konstanz) *Border-region treatment in the field-adapted adjustable density matrix assembler*
17:35 – 17:55	**E. Kordel** (Universität Karlsruhe) *Analytic energy gradients for the MP2-R12 method*
18:00 – 20:00	Dinner
20:00 – 23:00	Poster

Tuesday, 27 June 2006

09:00 – 09:50	**F. Furche** (Universität Karlsruhe) *RPA type correlation energy functionals*
09:50 – 10:25	**C. Hättig** (Ruhr-Universität Bochum) *Coupled-cluster response theory with linear r_{12} corrections*
10:25 – 10:45	**S. Pittalis** (FU Berlin) *Current spin density functional theory using orbital functionals*
10:45 – 11:15	Coffee
11:15 – 12:05	**F. Manby** (University of Bristol) *Recent advances in explicitly correlated electronic structure theory*
12:05 – 12:40	**T. Fleig** (Universität Düsseldorf) *Development of a relativistic 4-component multi-reference coupled cluster method*
13:00 – 14:30	Lunch
14:30 – 15:20	**M. Head-Gordon** (University of California, Berkeley) *Fast computational methods for strongly correlated electrons: Status, challenges and recent applications*
15:20 – 15:55	**C. Ochsenfeld** (Universität Tübingen) *Rigorous integral estimates for linear-scaling electron correlation methods*
15:55 – 16:25	Coffee
16:25 – 17:15	**M. Nooijen** (University of Waterloo) *Parameterized single reference coupled cluster theory*
17:15 – 17:35	**M. Hanrath** (Universität Köln) *Perturbative and connectivity analysis of MRexpT*
17:35 – 17:55	**M. Nest** (Universität Potsdam) *Correlated many electron dynamics with the multi-configuration time-dependent Hartree-Fock (MCTDHF) method*
18:00 – 20:00	Conference Dinner

Wednesday, 28 June 2006

09:00 – 09:50	**G. Kresse** (Universität Wien) *Beyond the local density approximation: hybrid functionals and GW*
09:50 – 10:25	**U. Birkenheuer** (MPI für Physik komplexer Systeme, Dresden) *Quantum chemical approaches for electron correlation in solids*
10:25 – 10:45	**T. Scott** (RWTH Aachen) *Minimization of the node-location error in diffusion quantum Monte Carlo*
10:45 – 11:15	Coffee
11:15 – 12:05	**R. J. Harrison** (Oak Ridge National Laboratory) *If you're not scared, you're not thinking big enough*
12:05 – 12:40	**M. Dolg** (Universität Köln) *The Hartree-Fock-Wigner model for electron correlation – Implementation and first results for molecules*
13:00 – 14:30	Lunch
14:30	Departure

Posters

P-1 **T. B. Adler** (Universität Stuttgart)
Application of local explicit correlation methods to chemical reactions

P-2 **S. R. Chinnamsetty** (MPI für Mathematik in den Naturwissenschaften, Leipzig)
Tensor product approximations in quantum chemistry

P-3 **B. Doser** (Universität Tübingen)
Linear-scaling AO-MP2 by rigorous integral screening

P-4 **R. Ermrich** (TU Dresden)
Influence of an electric field on the optical properties of selected organic molecules - a DFT based study

P-5 **R. Fondermann** (Universität Köln)
The Hartree-Fock-Wigner model for electron correlation – Implementation and first results for molecules

P-6 **C. Friedrich** (Forschungszentrum Jülich)
All-electron GW approximation in the augmented-plane-wave basis-set limit

P-7 **N. Gaston** (MPI für Physik komplexer Systeme, Dresden)
Lattice structure of mercury: Influence of electronic correlation

P-8 **E. Goll** (Universität Stuttgart)
DFT/CC methods applied to van-der-Waals systems

P-9 **A. W. Götz** (Universität Erlangen-Nürnberg)
An exact-exchange time-dependent density-functional method for molecules

P-10 **M. E. Harding** (Universität Mainz)
Parallelization of CCSD and CCSD(T) energies, gradients and second derivatives

P-11 **M. Heckert** (Universität Mainz)
Additivity scheme for equilibrium geometries based on coupled-cluster calculations combined with basis-set extrapolation techniques

P-12 **H. Jiang** (Universität Frankfurt)
Orbital-dependent representation of the correlation energy functional: Properties of second order Kohn-Sham perturbation expansion

P-13 **D. Ködderitzsch** (Ludwig-Maximilians-Universität München)
A relativistic extension and efficient implementation of the non-local coherent potential approximation within the multiple-scattering KKR method

P-14 **D. Ködderitzsch** (Ludwig-Maximilians-Universität München)
Implementation of a relativistic OPM method and application to free atoms

P-15 **D. S. Lambrecht** (Universität Tübingen)
Multipole-based integral estimates for the rigorous description of distance dependence in two-electron integrals

P-16 **N. N. Lathiotakis** (FU Berlin)
Reduced density matrix functional theory for periodic systems: Functionals and applications

P-17 **R. A. Mata** (Universität Stuttgart)
Accurate prediction of activation enthalpies in enzymes using local correlation Methods

P-18 **T. Metzroth** (Universität Mainz)
Perfo9rmance of decomposition schemes for orbital energy denominator like quantities

P-19 **G. Moritz** (Eidgenössische Technische Hochschule Zürich)
Convergence characteristics of quantum chemical density-matrix renormalization group (DMRG) calculations

P-20 **C. Neiss** (Forschungszentrum Karlsruhe)
Explicitly-correlated coupled-cluster methods for nonlinear properties

P-21 **M. Springborg** (Saarland-Universität Saarbrücken)
Efficient method for calculating the response of infinite periodic systems to finite electric fields

P-22 **M. Taut** (IFW Dresden)
Jahn-Teller-effect in the Wigner crystal in quantum dots in a magnetic field

P-23 **V. Tevekeliyska** (Saarland-Universität Saarbrücken)
Structural and electronic properties of sodium clusters with up to 60 atoms

P-24 **E. Voloshina** (MPI für Physik komplexer Systems, Dresden)
The method of increments for metals: Generating and testing of localized orbitals