Modern and Universal First-principles Methods for Many-electron Systems in Chemistry and Physics

Report on the Scientific Priority Program 1145
of the German Science Council

SPP 1145

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2 Overview

In 2002 the German Science Council (DFG, Deutsche Forschungsgemeinschaft) established the scientific priority program 1145 (SPP 1145, Schwerpunktprogramm 1145) *Modern and Universal First-principles Methods for Many-electron Systems in Chemistry and Physics*. The goal of the initiative is to bring together specialists for all aspects of first-principles electronic structure theory, e.g., quantum chemistry, theoretical physics as well as applied mathematics, and especially to encourage the development of new approaches. After the first symposium and review panel meeting June 1 - 3, 2003, in Bonn (organization: M. Dolg) financial support for 27 research projects was granted by the DFG. The second symposium of the SPP 1145, without review panel meeting, was held May 24 - 25, 2004 in Bonn (organization: B. A. Heß †) and covered nearly all branches of research carried out in the SPP 1145. At the third symposium and second review panel meeting July 4 - 6, 2005 in Bonn (organization: M. Dolg) 24 out of the 27 projects granted for the first financing period handed in a renewal proposal and 10 new project proposals were made. A total of 27 projects were granted financial support for the second financing period.[1] The fourth symposium, without review panel meeting, took place June 26 - 28, 2006, in Bad Herrenalb (organization H.-J. Werner, J. Gauss) and focussed mainly on wavefunction-based electronic structure methods. All four symposia were financed directly by the DFG. Conference programmes as well as lists of participants for the third and fourth symposium are given in section 6.1. (For information on the first and second symposium cf. the 2005 report on the SPP 1145.)

The 2007 symposium with review panel meeting for the last financing period of the SPP 1145 will again be held in Bonn, July 4 - 6, 2007 (organization: M. Dolg). Out of the 27 projects of the second financing period 22 ask for a renewal. In addition 4 new proposals were handed in.

In addition to the symposia workshops were organized on specialized topics, i.e., *Numerical Analysis in Quantum Chemistry* (2004 in Kiel; organizers: R. Schneider, W. Hackbusch, B. Hartke), *Orbital Functionals for Exchange and Correlation* (2005 in Berlin; organizers: S. Kurth, E. K. U. Gross, H. Ebert), *First Principles Approaches to Optical and Photoelectron Spectra* (2006 in Munich; organizers: H. Ebert, E. K. U. Gross, C. Ambrosch-Draxl, E. Molinari) and *Highly Accurate Calculations of Molecular Electronic Structure* (2007 in Bad Herrenalb; organizer: W. M. Klopper). These organized meetings enabled and enhanced the exchange of ideas between scientists from different branches of electronic structure theory, which in some cases resulted in new common projects. Programmes as well as lists of participants for the 2006 and 2007 workshops are given in section 6.2. (For information on the first and second workshop cf. the 2005 report on the SPP 1145.)

Three workshops with topics related closely to the SPP 1145 were organized by members of the priority program. These workshops did not request financial support and thus

[1] The project of Thomas Exner (Konstanz) joined the SPP 1145 following a decison of the DFG. The projects of Burkhard Fricke and Günther Plunien were taken out of the SPP 1145, but received the standard funding from the DFG.

are only briefly memtionned here. H.-J. Flad, R. Schneider organized a workshop *Pseudodifferential Calculus with Singularities, and Applications in Quantum Chemistry* February 27, 2006, at the Univerity of Potsdam. R. Schneider, W. Hackbusch, H.-J. Flad together with H. Yserentant organized a workkshop *Approximation in High Dimensions and the Electronic Schrödinger Equation* June 29 - July 1, 2006, at the University of Kiel. U. Birkenheuer, B. Paulus and M. Schütz organize together with C. Pisani a workshop *Local Correlation Methods: From Molecules to Crystals* September 12 - 15, 2007, at the Max-Planck-Institute of Physics of Complex Systems in Dresden.

A total number of **67** publications in international peer-reviewed journals appeared since 2005 from the research carried out within the SPP 1145 (2005: 21; 2006: 30; 2007: 16). An additional **12** manuscripts for international peer-reviewed journals are currently in press or accepted for publication and further **11** manuscripts have been submitted to these (status of July 1, 2007). Additional articles were published in books or are currently available from preprint servers. As it was expected, an increased publication activity of essentially all groups was observed during the second financing period. A list of publications is given in section 5.

Beate Paulus (Dresden) completed her Habilitation at the University of Regensburg end of 2005 on the topic of incremental calculations of correlation energies. Markus Reiher obtained a professorship at the ETH Zürich in 2006 and will not take part in the application process for the third funding period, thus the field of density matrix renormalization group techniques within the priority program is weakened. Christoph van Wüllen received an offer for a W3 professorship at the University of Kaiserslautern in 2007.

Martin Albrecht decided to abandon his research activities and to start a new career in industry early in 2006. Uwe Birkenheuer decided to leave the field of electronic structure calculations and obtained a position at the Institute of Safety Research at the Research Center Rossendorf near Dresden end of 2006. As a consequence the area of wavefunction-based investigations of band structures and excitons in crystalline systems is no more represented within the priority program.

The present report briefly summarizes the development and activities of the SPP 1145 for the second financing period, i.e. for the period between the third and the upcoming fifth symposium. For reasons of brevity (as well as technical difficulties, i.e. a broken finger on the right hand of the coordinator) a listing of conference attendances, travels of scientists from the SPP 1145 to visit other groups as well as guests in participating groups financed by the priority program are not included in the present report. Additional information is available on the homepage of the SPP 1145, i.e., http://www.uni-koeln.de/spp1145.

3 Participants and Projects

3.1 First financing period 2003-2005

1. *Local ab initio schemes to describe excitons in polymers and solids*
   Martin Albrecht (Siegen) Al 625/1-1
2. *Wave-function-based correlation method for ground states and excited electron hole and attachment states of periodic systems*
   Uwe Birkenheuer (Dresden) Bi 822/1-1
3. *Wannier-type orbital based Hartree-Fock (-Wigner) electronic structure theory and wavefunction-based correlation treatment for periodic systems*
   Michael Dolg (Köln) Do 440/6-1
4. *Relativistic Optimized Potential Method for magnetic solids*
   Hubertus Ebert (München) Eb 154/13-1
5. *Density functional theory with implicit functionals: Correlation energy*
   Eberhard Engel (Frankfurt) En 265/4-1
6. *Orbital magnetism in molecules and solids*
   Helmut Eschrig, Gotthard Seifert and Manuel Richter (Dresden) Es 85/10-1 and Se 651/28-1
7. *Development of a Relativistic Hilbert-Space Multi-Reference Coupled-Cluster Program*
   Timo Fleig (Düsseldorf) Fl 356/2-1
8. *Accurate wave functions for open-shell atoms including open d- and f-shell elements*
   Stephan Fritzsche (Kassel) Fr 1251/11-1
9. *Spin-adapted coupled-cluster theory for the treatment of low-spin open-shell states*
   Jürgen Gauß (Mainz) Ga 370/4-1
10. *Concepts from the optimized potential method and orbital-dependent kernels in time-dependent density-functional theory*
    Andreas Görling (Bonn, since 2004 Erlangen) Go 523/13-1
11. *A dimension-adaptive sparse grid method for the Schrödinger equation*
    Michael Griebel (Bonn) Gr 1144/12-1
12. *Development of a reduced-density-matrix functional theory for solids*
    Eberhard K. U. Groß (Berlin) Gr 1267/7-1
13. *Development and application of explicitly-correlated coupled-cluster methods for non-linear optical properties*
    Christof Hättig, Willem Marten Klopper (Karlsruhe) Ha 2588/3-1
14. *Development and application of quantum-chemical density-matrix renormalization group methods*
    Bernd A. Heß † (Bonn), continued by Markus Reiher (Bonn, since 2005 Jena) He 1553/7-1

15. *Development and implementation of modern density functional methods for property calculations*
    Martin Kaupp (Würzburg) Ka 1187/6-1
16. *Development, implementation and application of the analytical calculation of energy derivatives, especially nuclear gradients, of electron-correlation methods employing wavefunctions that depend explicitly on the interelectronic distances*
    Willem Maarten Klopper (Karlsruhe) Kl 721/2-1
17. *Development and investigation of orbital functionals in density- and current- density functional theory*
    Stefan Kurth (Berlin Ku 1126/3-1
18. *Development of electron structure quantum Monte Carlo methods*
    Arne Lüchow (Aachen) Lu 588/7-1
19. *One- to four-component correlated relativistic electronic structure methods based on density matrix renormalization group techniques*
    Markus Reiher (Bonn, since 2005 Jena) Re 1703/1-1
20. *Ab initio electron dynamics with the multi-configuration (explicitly) time- dependent Hartree-Fock (MCTDHF) method*
    Peter Saalfrank (Potsdam) Sa 547/6-1
21. *First-principle method for the calculation of magnons in real materials*
    Leonid M. Sandratskii (Darmstadt) Sa 798/2-1
22. *Electronic structure and excitation spectra of magnetic materials within first- principles many-body perturbation theory*
    Arno Schindlmayr, Gustav Bihlmayer and Stefan Blügel (Jülich) Schi 570/3-1
23. *Operator calculus of density matrices and sparse wavelet representations*
    Reinhold Schneider (Kiel), Wolfgang Hackbusch and Heinz-Jürgen Flad (Leipzig) Schn 530/4-1 and Ha 1324/24-1
24. *Development of local electron correlation methods for periodic systems*
    Martin Schütz (Stuttgart, since 2004 Regensburg) Schu 1456/3-1
25. *Constructing density functionals compatible with exact exchange, utilizing the strong interaction limit*
    Michael Seidl (Regensburg)
26. *Ab initio QED calculations of spectra and transition probabilities in atomic few-electron systems*
    Gerhard Soff † (Dresden), continued by Günther Plunien (Dresden) So 333/17-1
27. *Coupling of density-functional and configuration-interaction-type methods*
    Hermann Stoll and Heinz-Joachim Werner (Stuttgart) Sto 305/3-1

3.2 Second financing period 2005-2007

1. *Local ab initio schemes to describe excitons in polymers and solids*
   Martin Albrecht (Siegen) Al 625/1-2
2. *Wave-function-based correlation method for ground states and excited electron hole and attachment states of periodic systems*
   Uwe Birkenheuer (Dresden) Bi 822/1-2
3. *Wannier-type orbital based Hartree-Fock (-Wigner) electronic structure theory and wavefunction-based correlation treatment for periodic systems*
   Michael Dolg, Michael Hanrath (Köln) Do 440/6-2
4. *Relativistic Optimized Potential Method for magnetic solids*
   Hubertus Ebert (München) Eb 154/13-2
5. *Density functional theory with implicit functionals: Correlation energy*
   Eberhard Engel (Frankfurt) En 265/4-2
6. *Orbital magnetism in molecules and solids*
   Helmut Eschrig, Gotthard Seifert and Manuel Richter (Dresden) Es 85/10-2 and Se 651/28-2
7. *Test and Improvement of Current Density Functionals using an exactly solvable two-electron model*
   Helmut Eschrig and Manuel Richter (Dresden) Es 85/11-1
8. *Optimization of Fragment Electron Densities for the Usage in Mixed Quantum Mechanical / Molecular Mechanical (QM/MM) and Fragment-Based Quantum Mechanical Methods*
   Thomas Eckart Exner (Konstanz) Ex 15/8-1
9. *Development of a Relativistic Hilbert-Space Multi-Reference Coupled-Cluster Program*
   Timo Fleig (Düsseldorf) Fl 356/2-2
10. *Concepts from the optimized potential method and orbital-dependent kernels in time-dependent density-functional theory*
    Andreas Görling (Erlangen-Nürnberg) Go 523/13-2
11. *A dimension-adaptive sparse grid method for the Schrödinger equation*
    Michael Griebel (Bonn) Gr 1144/12-2
12. *Development of a reduced-density-matrix functional theory for solids*
    Eberhard K. U. Groß (Berlin) Gr 1267/7-2
13. *Operator calculus of density matrices and sparse wavelet representations*
    Wolfgang Hackbusch (Leipzig), Reinhold Schneider (Kiel), Heinz-Jürgen Flad (Leipzig) Ha 1324/24-2 and Schn 530/4-2
14. *Development and application of explicitly-correlated coupled-cluster methods for non-linear optical properties*
    Christof Hättig (Karlsruhe, since 2006 Bochum), Willem Marten Klopper (Karlsruhe) Ha 2588/3-2

15. *Development, implementation and application of the analytical calculation of energy derivatives, especially nuclear gradients, of electron-correlation methods employing wavefunctions that depend explicitly on the interelectronic distances*
Willem Marten Klopper (Karlsruhe) Kl 721/2-2

16. *Development and investigation of orbital functionals in density- and current- density functional theory*
Stefan Kurth (Berlin) Ku 1126/3-2

17. *Development of electron structure quantum Monte Carlo methods*
Arne Lüchow (Aachen) Lu 588/7-2

18. *Development of a linear-scaling MP2 method for large molecules by rigorous integral criteria*
Christian Ochsenfeld (Tübingen) Oc 35/3-1

19. *Development of a wavefnction-based ab initio method for metals applying the method of increments*
Beate Paulus (Dresden) Pa 1360/1-1

20. *Development and application of quantum chemical density matix renormalization group methods*
Markus Reiher (Bonn, since 2005 Jena, since 2006 Zürich) Re 1703/1-2

21. *Ab initio electron dynamics with the multi-configuration (explicitly) time- dependent Hartree-Fock (MCTDHF) method*
Peter Saalfrank and Tilman Klamroth (Potsdam) Sa 547/6-2

22. *Electronic structure and excitation spectra of magnetic materials within first- principles many-body perturbation theory*
Arno Schindlmayr, Gustav Bihlmayer and Stefan Blügel (Jülich) Schi 570/3-2

23. *Development of local electron correlation methods for periodic systems*
Martin Schütz (Regensburg) Schu 1456/3-2

24. *Development and implementation of theoretical methods for dealing with functions of the quantum mechanical operator r in extended systems*
Michael Springborg (Saarbrücken) Sp 439/20-1

25. *Coupling of density-functional and configuration-interaction-type methods*
Hermann Stoll (Stuttgart) Sto 305/3-2

26. *Local explicit correlation methods*
Hans-Joachim Werner (Stuttgart) We 984/15-1

27. *Development of an efficient and quasirelativistic two-component program package for Hartree-Fock and density functional calculations*
Christoph van Wüllen (Berlin) Wu 288/4-1

4 Scientific Results

The following paragraphs give a brief overview over the most important scientific aspects of the projects carried out by the research groups in the framework of the SPP 1145. The text is based on summaries provided by the project leaders as far as they have been provided until July 1, 2007. For further details cf. the individual reports/applications to the DFG as well as the publications listed below.

One part of the project of **M. Dolg**, **M. Hanrath** and their coworkers deals with the implementation and improvement of the Hartree-Fock-Wigner correlation model advocated by P. Gill. First results for bond lengths, binding energies and dissociation energies of diatomic molecules with light atoms have been presented. The correlation kernel symmetric in the interelectronic distance and relative momentum was found not to lead to satisfactory results, although an accuracy similar to the Lee-Yang-Parr correlation energy density functional was observed. An extension to an asymmetric correlation kernel lead only to small improvements. At present a coupling of the Hartree-Fock-Wigner model to multiconfiguration self-consistent field calculations is explored. The second part of the project lead to the implementation of a fully automatized calculation of correlation energies at the coupled cluster singles and doubles level within the so-called incremental scheme devised by H. Stoll. The C++ code is parallelized and can handle expansions for molecules as well as periodoc systems to any order. Using this tool the convergence and the error propagation of the incremental series was investigated for a large number of systems exhibiting significant differences in their electronic structure. The evaluation of properties using the incremental expansion was also investigated. Future goals are improvements of the computational efficiency of the approach, the derivation and implementation of expansions especially suited for e.g. the calculation of energy differences, the evaluation of energy gradients wrt the nuclear positions as well as the extension to size-extensive correlation schemes other than coupled cluster singles and doubles.

The first part of the project of **H. Ebert** and his group aims at an implementation of the relativistic version of the optimised potential method (ROPM) for spin-polarised systems working with the four-component Dirac formalism. For this purpose three variants of the ROPM equations have been developed in terms of the Green's function supplying a common platform to deal with bound states as well as itinerant states in solids. After having solved several delicate numerical problems a robust and efficient implementation for atomic open-shell systems could be achieved. Comparison with LDA as well as non-relativistic OPM results revealed the impact of the use of an orbital dependant functional and relativistic effect, respectively, as reflected e.g. by the hyperfine fields. Based on the experience made for the atom case, a corresponding implementation for the solid could be achieved recently as well. First applications aimed at the impact of the ROPM-scheme on the band gap of semiconductors and the magnetic properties of ferromagnets. The second part of the project was devoted to an implementation of the dynamical mean field theory (DMFT), again within the framework of the Dirac formalism and using the Green's function technique. The latter feature allowed, in particular, the application to systems without Bloch symmetry as impurities and disordered alloys. Application to photo emission spectroscopy allowed for the first time to deal with matrix element effects and

correlations via the DMFT on a common platform. These calculations led to appreciable improvements with respect to LDA-calculations when comparing the results to experiment. To account for the impact of correlation effects on the spin-orbit induced orbital moments a generalised DMFT-solver was developed on the TMA (T-matrix approximation) level. Again, shortcomings of the LDA could be removed or at least reduced. First steps to extend the single-site DMFT scheme used so far to a cluster version were done. As a spin-off this led to an efficient implementation of the non-local coherent potential approximation (NLCPA) alloy theory. Application to calculations of the residual resistivity of disordered alloys demonstrated for the first time the impact of ordering in a convincing way.

In response to the overestimation of correlation effects by the most basic orbital-dependent correlation functional $E_c^{(2)}$ (Phys. Rev. A 72 (2005) 052503, J. Chem. Phys. 123 (2005) 224102) derived from second order Kohn-Sham perturbation theory, two types of partial resummations of the perturbation series have been studied by **E. Engel** and coworkers. The technically simplest form resums the hole-hole Epstein-Nesbet diagrams. The resulting correlation functional improves correlation energies and potentials significantly, and turns out to be variationally stable for all neutral and singly ionized atoms up to Ar (in contrast to $E_c^{(2)}$) (J. Chem. Phys. 125 (2006) 184108). As the simplest functional including screening in a systematic fashion, we have also implemented the RPA. Lacking the second order exchange (SOX) contribution, this functional overestimates correlation effects substantially. On the other hand, the combination of the RPA both with a 'screened' SOX term and with the LDA for all correlation effects beyond the RPA gives rather accurate results. We have also demonstrated that the frozen core approximation, in which only virtual excitations of the valence electrons are taken into account, provides an accurate correlation potential v_c in the complete valence regime, i.e. whereever v_c is relevant (Int. J. Quantum Chem. 106 (2006) 3242). In addition, several collaborations within the SPP 1145 have been pursued during the second period (Phys. Rev. B 74 (2006) 045119).

One project in the group of **H. Eschrig** and **M. Richter (Dresden)** deals with exactly solvable few electron systems in a tunable parabolic confinement (frequency ω) and magnetic field $\mathbf{B}$. This model (realised in quantum dots) allows the investigation of correlations for tunable correlation strength including the strong – (Wigner molecule) and the weak correlation (one electron) limit. The *two* electron system is analytically solvable for an infinite, but discrete set of external parameter values. For this system, we made progress in constructing the exact XC potentials V_{xc} and $\mathbf{A}_{xc}$ in CDFT using the exact spin – and current densities from the analytical solutions. The next envisaged step is the comparison of the exact potentials with the LDA results. Results will be ready for publication presumably in half a year. For the *three* electron system exact solutions could be found only in the strong-correlation limit. These solutions reveal a Jahn-Teller distortion of the Wigner molecule, which depends on the total spin S and orbital angular momentum L (cf. publications). In the ground state, the Wigner molecule forms an equilateral triangle (as expected from naive reasoning) only, if the state is a quartet ($S = 3/2$) and the orbital angular momentum is a magic quantum number ($L = 3m, m = integer$). Otherwise the triangle is isosceles. For $L = 3m + 1$ one of the sides is longer and for $L = 3m - 1$ one of the sides is shorter than the other two.

The group of **T. Exner** is developing a fragment-based quantum chemical method for large biomolecules. The specific aim of the project started January 2006 was to optimize the obtained fragment electron densities. When dividing a large macromolecule into smaller fragments, covalent bonds must be broken and the free valences must be filled, which should lead to the least possible perturbation. This problem is also known from mixed quantum mechanical / molecular mechanical approaches. It could be shown that using hybrid orbitals as proposed in the generalized hybrid orbital (GHO) method by Pu et al. can, compared to hydrogen capping atoms, largely improve the fragment electron densities and, in this way, the calculated total energies of the macromolecule (Z. Phys. Chem. 220, 927-944, 2006). Therefore, this method is developed further to make it applicable to a large number of problems. But the capping atom approach can also be improved by using atoms with a specially designed effective core potential, which is also tried in current investigations.

The major achievement of the group of **T. Fleig** in the preceding application period was the completion of a 4-component general-order multi-reference coupled cluster method (Theor. Chem. Acc., in press) capable of employing any Hamiltonian implemented in the local development versions of the `DIRAC` program package. In particular, this includes the fully relativistic Dirac-Coulomb, the infinite-order two-component (Jensen and M Iliaš) including the Gaunt (spin-other-orbit) term, the 4-component spin-orbit free, and the non-relativistic Levy-Leblond Hamiltonians. With this implementation we are now able to treat complicated bonding situations in general (heavy-element) molecules, dissociation problems, and other cases which require a multi-reference ansatz, and we may in particular include spin-orbit interaction rigorously. The current algorithm is based on intermediate configuration interaction expansions which reduces the efficiency in terms of an increased scaling of the method with system size. We are currently implementing the more efficient commutator-based algorithm with an optimal scaling in accord with standard coupled cluster methods.

As a prerequisite for a time-dependent density-functional method based on the nonadiabatic exact exchange kernel (EXX-TDDFT method) the long standing problem of finding, within a Gaussian basis set framework, a numerical stable optimized potential method that represents a proper Kohn-Sham method was solved by introducing such a method by the group of **A. Görling**. The new method not only is numerical stable but in addition efficient, easy to implement, and does not require any numerical integrations as standard Kohn-Sham methods do. Concerning the development of an EXX-TDDFT method, a first test implementation yielded very promising results indicating that EXX-TDDFT methods can solve the problem of conventional TDDFT methods to describe charge-transfer excitations.

In the first and second period of the SPP 1145, the group of **M. Griebel** developed and implemented our sparse grid product methods for the discretization of Schr"odinger's equation with different choices of multi-level bases. Here, a Fourier basis, a wavelet basis, and a basis with almost orthonormal multiscale functions using Gaussians were employed. These approaches were then used to compute one-dimensional model systems with several particles and first small three-dimensional systems up to the lithium atom. The Gaussian

multiscale basis leads to the best constants and indeed delivers the convergence rates expected in presence of the electron-electron cusp. For the third financing period, it is planned to further improve the method, and to apply it to several small molecules with up to 10 electrons, such as He_2, LiH, CH, Be_2, and H_2O. Here, an improved multilevel eigenvalue solver for large near-degenerate systems, an a priori matrix compression scheme to exploit a new variant of generalized Slater-Condon rules, and a generalized basis including explicit two-particle correlation factors will be of special importance.

In the group of **E. K. U. Gross** the development and application of reduced-density-matrix-functional theory (RDMFT) was further pursued. One aspect was the calculation of the fundamental gap through the discontinuity of the chemical potential for functionals of the one-body reduced-density matrix (1-RDM). It was found that the removal of self interaction is an essential ingredient of these functionals in order to properly represent the discontinuity. While the first implementation of RDMFT for solids was based on Wannier functions, a new Bloch-state implementation has been developed on the basis of the EXCITING FP-LAPW code. In order to construct functionals of the 1-RDM for solids, both metallic systems and insulators have to be properly described. The performance of a number of functionals was tested for a prototype metal: the uniform electron gas. It turned out that the most recent generation of functionals (which so far was only known to perform well for molecules) are also superior in reproducing the correlation energy of the uniform gas. Furthermore, a novel functional was designed such as to reproduce EXACTLY the correlation energy of the electron gas. This functional was subsequently applied to finite atomic and molecular systems with very encouraging results. The functional was found to correctly describe the dissociation of closed-shell diatomic molecules into open-shell fragments. Hence this functional works well in two extreme limits: the uniform gas and the dissociation of molecules. Finally, a detailed assessment of a number of RDMFT-functionals was performed on the G2 test set. The best functionals were found to be as accurate as MP2 theory.

In the project by **C. Hättig** and **W. Klopper** on the development of CC-R12 response methods, the problem of an unbalanced description of the ground and excited states with the standard choice of the R12 geminal functions have been overcome by implementing a generalized orbital subspace for their construction (J. Chem. Phys. 125, 064111 (2006)). The implementation of CC-R12 response theory has been extended from CC2-R12 to CCSD(R12) for excitation energies and the linear, quadratic and cubic response functions. First results for frequency-depending polarizabilities and first and second hyperpolarizibilities are promising and indicate that the R12 ansatz improves the convergence of these properties with the one-electron basis sets to a similar extend as it does for ground state total energies (J. Chem. Phys. 126, 154101 (2007)). As a first step towards an extension of the present implementation to so-called ansatz 2 of R12 theory and the recently introduced improved correlation factors, an implementation of the CCSD(F12) model for ground state energies has been developed (Phys. Chem. Chem. Phys. 9, 1921 (2007)).

The group of **W. Klopper** has implemented analytical nuclear gradients in the DALTON program at the level of explicitly correlated second-order Møller–Plesset perturbation theory (MP2-R12). The implementation has been accomplished for standard approxima-

tion A using a resolution-of-the-identity auxiliary basis that is restricted to be identical to the orbital basis. The gradients can be computed with and without frozen core. To test the new implementation, the geometries of nine stationary points on the potential energy surface of the water dimer have been optimized near to the basis set limit of MP2 theory and the results are compared with earlier studies. In future work, the analytical calculation of nuclear gradients shall be implemented in the TURBOMOLE program for the DF-MP2-R12 version of MP2-R12 theory that uses a complementary auxiliary basis set (CABS), a linear combination of Gaussian geminals in place of the linear r_{12} term, and various approximations to the integrals over the commutator of the kinetic energy operator with the geminals.

During the past funding period **S. Kurth** and coworkers completed the implementation of the Optimized Effective Potential (OEP) method in the context of current-density functional theory (CDFT) both for finite and extended systems. For open-shell atoms they found small but insufficient improvement for the spurious energy splittings of degenerate ground states as compared to spin-DFT while for quantum dots in external magnetic fields excellent agreement with Quantum-Monte-Carlo results was achieved provided that the exact exchange functional is used together with LDA correlation. The implementation for extended systems was done in a way to allow for the description of non-collinear magnetism. It was found that, using the same orbital functional, spin-DFT and CDFT results for spin-orbit induced band splittings and orbital magnetic moments are extremely similar. They also showed that, unlike for non-collinear LDA, for orbital functionals the magnetization density and the exchange-correlation part of the effective magnetic field are not necessarily locally parallel. This fact might be crucial to properly describe magnetization dynamics. Finally, Kurth and coworkers have constructed a current-dependent extension of the Colle-Salvetti correlation energy functional which in combination with exact exchange recovers the degeneracy between different ground states of open-shell atoms.

A. Lüchow and coworkers have extended the quantum Monte Carlo method to calculate Rydberg states in collaboration with A. Görling and F. della Sala. The analysis of the nodal regions revealed in some cases an unbalanced calculation of energies in standard diffusion Monte Carlo (DMC) that has been overcome with a new weighted DMC algorithm. The DMC energy depends only on the accuracy of the nodal hypersurface. In this project, a local property depending on the accuracy of the nodal hypersurface has been developed, allowing the assessment of the accuracy locally. Furthermore, a simple mean of this property has been developed as a measure for the accuracy of overall nodal hypersurface. With minimization of this mean the first direct optimization of the nodal hypersurface of simple multideterminant wave functions of the Be atom and the C_2 molecule has been successful.

The group of **C. Ochsenfeld** focuses on the development of a linear-scaling MP2 method for large molecules. The key feature are multipole-based integral estimates (MBIE), which account for the 1/R coupling in two-electron integrals and allow to rigorously preselect integral products in AO-MP2 theory. Here, the magnitude of products decays at least with $1/R^4$, so that a linear-scaling behavior can be achieved by numerical thresholding without sacrificing any accuracy. The linear-scaling increase of the computational effort is reached much earlier than for HF or DFT approaches: e.g. the exact

behavior indicates a scaling of $N^{1.0}$ from one to two DNA base-pairs for a 6-31G* basis. The number of significant elements in the pseudo-density matrices and of shell pairs hints to a very similar linear-scaling behavior for larger basis sets studied up to cc-pVQZ. First results of a preliminary implementation show that an early crossover to conventional MP2 schemes below two DNA base pairs is observed. Furthermore, already for a system with four DNA base pairs wins in the order of one to two orders of magnitude are expected.

M. Nest, P. Saalfrank and coworkers implemented the Multi-Configuration Time-Dependent Hartree-Fock (MCTDHF) method, also denoted as TD-CASSCF, and used it to simulate the explicitly time-dependent, correlated many electron dynamics in model systems, and in real molecules. The program, which consists by now of ca 6000 lines of code, has been interfaced with the GAMESS quantum chemistry package, for the calculation of integrals of Gaussian Type Orbitals. A large number of computational tests have been performed, like a comparison of various propagation schemes, complex absorbing potentials for the treatment of ionization in one-dimensional model systems, and propagation in imaginary time to determine the electronic ground state of molecules. The scaling behaviour (computation time as a function of the number of electrons), and the limits of TD-CASSCF, namely TD Hartree-Fock and TD Full CI have been examined. Further, by combining MCTDHF with Heller's wave packet approach to spectroscopy, they were able to calculate vertical excitation spectra quantitatively, and oscillator strengths and transition dipole moments qualitatively, for small molecules such as lithium hydride and methane. In parallel to this, the TD Configuration Interaction method, so far restricted to single excitations (TD CIS) or perturbative inclusion of double excitations (TD CIS(D)), was extended to explicitly include double excitations. TD CI was applied to intramolecular charge transfer in larger molecules, Li-$(Ph)_n$-CN, with n up to 3. For the H_2 molecule, a TD Full CI solution was possible and benchmark calculations have been carried out to determine linear and nonlinear optical properties of the molecule in response to ultrashort laser pulses.

The group of **M. Schütz** works on local electron correlation methods for periodic systems. Numerous obstacles concerning the periodic density fitting scheme in DF-LMP2 had to be surmounted to make the new code a practical tool for real applications: Due to problems with the dipole correction in the context of low thresholds for PAO redundancies a new two-step DF scheme had to be developed. Furthermore, the algorithm for solving the LMP2 equations had to be re-designed which now makes it feasible to include larger numbers of orbital pairs in the calculations. An LMP2 correction to the density matrix (so far orbital-unrelaxed) for calculating Compton profiles, X-ray structure factors, charge distributions, *etc.* was also implemented. Finally, in the context of molecular adsorption on surfaces, a partitioning of the orbital pairs was introduced, which allows it to investigate such systems in an efficient way. Another project is the development of a local Coupled Cluster Linear Response method for the calculation of excited state properties of extended molecular systems. Excitation energies, first-order properties of ground and excited states, and oscillator strengths now can be calculated for extended molecules (< 100 atoms) in the framework of local CC2 response theory. A new scheme for domain specification based on the solutions of the CPHF and CPL (Coupled Perturbed Localization) equations

has been introduced, which is advantageous for property calculations. A semi-local CC2 response program has also been implemented, which now substitutes the CIS wavefunction for excited state domain specification.

A systematic derivation of orbital polarization corrections (OPC) from four-current density functional theory that has been found by the group of **G. Seifert** in the previous period and has been implemented in the full-potential local-orbital (FPLO) code and tested for different systems like Co impurities in Au, full-Heusler alloys, and a number of uranium compounds. It turned out that a variant of OPC with only exchange contributions performs better than the originally proposed variant for both uranium compounds and elemental 3d transition metals. This approach should be further tested and completed with non-collinear magnetization density calculations in the final period. We have also studied the orbital magnetism in quasi 1D systems (iron nanowires), using optimized structures of iron in nanotubes. The spin polarization effects within a collinear approach (SDFTB) has been tested extensively for the magnetic and structural properties of iron clusters. We have also developed a non-collinear extension of the spin-polarized density-functional based tight binding (SDFTB) expressions so that they are rotationally invariant with respect to changes in the quantization direction. This treatment was implemented into the SDFTB program and has been tested for the magnetic properties of small iron clusters.

The project of **B. Paulus** is the application of wavefunction-based quantum chemical correlation methods to metals via the method of increments. The correlation energy of the solid is expanded in terms of localized orbital groups and increments of these groups The main different to the incremental scheme for band-gap systems is the generation of localized orbitals in metals. We have developed an embedding scheme (J. Chem. Phys. 126, 134115, 2007), that can mimic the metallic band structure in a finite fragment of the solid and can generate localized orbital for a metal, which are transferable to the solid. A comparison of the many-body expansions of the correlation energy in free clusters compared to the embedded one (Mol. Phys. submitted 2007) shows, that only in the embedded clusters one can reach a converged series of the many-body expansion. The application of the developed method to ground-state properties of magnesium yields a very good agreement with experiments (Phys. Rev. B, in press, 2007). Due to the method development made within the SPP we can now reliably determine the structural properties of zinc and cadmium and explain the highly anisotropic hcp structure in the group 12 metals (collaboration with M. Jansen and U. Wedig, MPI-FKF Stuttgart).

The coupling of short-range density-functional (DFT) and long-range wavefunction-based ab-initio methods persued by the groups of **H. Stoll** and **H.-J. Werner** has been further extended by a) developing short-range spin-polarized LDA (co-operation with P. Gori-Giorgi and A. Savin, Paris), and GGA as well as meta-GGA functionals of the PBE and TPSS type, respectively; b) coupling these functionals with high-spin long-range RCCSD(T) calculations within the Molpro program package (co-operation with T. Leininger, Toulouse); c) implementing local-correlation schemes for the long-range part of the mixed scheme (co-operation with F. Manby, Bristol); d) systematically testing the mixed approach for van der Waals molecules and various other test sets of molecules (including the G2 set).

The aim of the project of **H.-J. Werner** (Stuttgart) is to improve the basis set convergence in local coupled cluster methods by including r_{12}-dependent correlation factors. The methods should be applicable to molecules with 50-100 atoms and yield accurate results with medium-size basis sets. In the current funding period explicitly correlated MP2-F12 methods based on closed-shell and spin-restricted open-shell shell Møller-Plesset perturbation theory were developed. A systematic hierarchy of approximations was implemented and extensively tested (J. Chem. Phys. 126 (2007) 164102). It was shown that with basis sets of triple zeta quality (aug-cc-pVTZ) about 99% of the basis set limit of the MP2 correlation energy can be revovered, and the correlation contributions to reaction energies, ionization energies, electron affinities, as well as interaction energies of molecular clusters can be obtained with an accuracy that is in all cases better than that of standard MP2 with aug-cc-pV5Z basis sets. These methods were combined with local approximations (J. Chem. Phys. 124 (2006) 094103) and this made it possible to perform LMP2-F12 calculations with up to 87 atoms and over 3100 basis functions (so far). The methods were applied to highly accurate calculations of reaction barriers in enyzmes (Angew. Chem. 118 (2006) 7010). Further ongoing applications concern highly accurate calculations for weakly bound systems and a more extensive study of reaction enthalpies for more than 50 chemical reactions. For the next funding period, the extension of these methods and applications to the coupled cluster level is planned.

In the group of **C. van Wüllen** the domain of quasirelativistic two-component calculations has been extended toward larger systems. This has been achieved partly by technicalities (improved parallelization) but mainly by the implementation of matrix elements for spin-dependent effective core potentials both for energy calculations and geometry gradients. This makes possible calculations with a large number of heavy (or even superheavy) atoms, so a pilot application on the adsorption of an element 113 atom on various gold clusters modeling gold surfaces has been done. This modeling is relevant for thermochromatography experiments used for the characterization of superheavy elements. The behaviour of eigenfunctions of quasirelativistic all-electron Douglas-Kroll operators in the vicinity of a point-nucleus has been investigated by special numerical techniques. It turns out that these eigenfunctions are not more singular than Dirac spinors, starting from second-order Douglas-Kroll. The claim, that these functions show a stronger singularity, is most likely only true for the "no-pair" (first-order Douglas-Kroll) operator.

5 Publications

The publications (status: published, in press, accepted or submitted) listed here summarize results obtained in their largest part or exclusively in the projects financed in the framework of the SPP 1145 or by scientists financed by the SPP 1145 during the years 2005 - 2007, roughly corresponding to the second financing period. Other publications on topics relevant to the SPP 1145, but not being a direct outcome of the SPP 1145 are not listed.[2]

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3. *Tailoring the induced magnetism in carbon-based and non-traditional inorganic nanomaterials*, A. N. Andriotis, R. M. Sheetz, N. N. Lathiotakis, M. Menon, Int. J. of Nanotechnology (2007) accepted.
4. *Rydberg states with quantum Monte Carlo.* A. Bande, A. Lüchow, F. Della Sala, A. Görling, J. Chem. Phys. 124 (2006) 114114.
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88. *Nodal Structure of Schrdinger Wave Function: General Results and Specific Models*, T. C. Scott, A. Lüchow, J. Phys. B 40 (2007) 851.
89. *The Blue Xe_4^+ Cation. Experimental Detection and Theoretical Characterization,* S. Seidel, K. Seppelt, C. van Wüllen, X. Y. Sun, Angew. Chem. (2007) accepted.
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91. *Comparison of exact-exchange calculations for solids in current-spin-density- and spin-density-functional theory*, S. Sharma, S. Pittalis, S. Kurth, S. Shallcross, J.K. Dewhurst, E.K.U. Gross, cond-mat/0704.0244.
92. *Fuzzy Fragment Selection Strategies, Basis Set Dependence, and HF - DFT Comparisons in the Applications of the ADMA Method of Macromolecular Quantum Chemistry*, Z. Szekeres, T.E. Exner, P.G. Mezey, Int. J. Quantum Chem. 104 (2005) 847.

93. *Jahn-Teller distortion of the Wigner molecule in a three-electron quantum dot and a magnetic field*, M. Taut, Physica E (to appear), (Proccedings for the EP2DS Meeting 2007 in Genova)
94. *Jahn-Teller distortion of the Wigner molecule in a three-electron quantum dot and a magnetic field: pair function approach*, M. Taut, H. Eschrig, M. Richter, Phys. Rev. A (manuscript ready for submission, available on request)
95. *Quintuple-ζ quality coupled-cluster correlation energies with tripe-ζ basis sets*, D. P. Tew, W. Klopper, C. Neiss, C. Hättig, Phys. Chem. Chem. Phys. 9 (2007) 1921.
96. *Fast local-MP2 method with Density-Fitting for crystals. B. Test calculations and application to the carbon dioxide crystal*, D. Usvyat, L. Maschio, F. R. Manby, S. Casassa, M. Schütz, C. Pisani, Phys. Rev. B (2007) submitted.
97. *Embedding procedure for ab initio correlation calculations in group II metals*, E. Voloshina, N. Gaston, B. Paulus, J. Chem. Phys. 126 (2007) 134115.
98. *Wavefunction-based ab initio method for metals: application of the incremental scheme to magnesium*, E. Voloshina, B. Paulus, Phys. Rev. B (2007) in press.
99. *Correlation energies for small Mg-cluster in comparison to bulk Mg*, E. Voloshina, B. Paulus, Mol. Phys. (2007) submitted.
100. *General Orbital Invariant MP2-F12 Theory*, H.-J. Werner, T. B. Adler, F. R. Manby, J. Chem. Phys. 126 (2007) 164102.
101. *Accurate and Efficient Treatment of Two-Electron Contributions in Quasirelativistic high-order Douglas-Kroll Density Functional Calculations,* C. van Wüllen, C. Michauk, J. Chem. Phys. 123 (2005) 204113.
102. *Numerical Instabilities in the Computation of Pseudopotential Matrix Elements,* C. van Wüllen, J. Comput. Chem. 27 (2006) 135.
103. *Gradients for Two-Component Quasirelativistic Methods. Application to dihalogenides of element 116,* C. van Wüllen, N. Langermann, J. Chem. Phys. 126 (2007) 114106.
104. *Evaluation of electronic correlation contributions for optical tensors of large systems using the incremental scheme.* J. Yang, M. Dolg, J. Chem. Phys. (2007) in press.

6 Symposia and Workshops

6.1 Symposia

The third symposium and second review panel meeting 2005 was held in Bonn. The fourth symposium was organized by Hans-Joachim Werner (Stuttgart) and Jürgen Gauss (Mainz) in 2006 in Bad Herrenalb. The fifth symposium and third review panel meeting will also take place in Bonn in 2007.

It is planned that the 2008 symposium will be organized by Hubert Ebert (München) and the final symposium 2009 by the SPP 1145 coordinator.

6.1.1 Symposium and review panel meeting 2003 (June 1 - 3, 2003, Bonn)

Organizer:

- Prof. Dr. Michael Dolg (Köln)

Number of participants: 56

In this initial symposium and review panel meeting 34 project applications were presented in short oral presentations of 10 minutes each (including discussion) as well as a poster session. Out of these 27 projects were selected for the first financing period of the SPP 1145.

6.1.2 Symposium 2004 (May 24 - 25, 2004, Bonn)

Organizer:

- Prof. Dr. Bernd Artur Hess † (Bonn)

Number of participants: 70

6.1.3 Symposium and review panel meeting 2005 (July 4 - 6, 2005, Bonn)

Organizer:

- Prof. Dr. Michael Dolg (Köln)

Number of participants: 90

34 project proposals were presented on posters, 24 being renewal proposals and 10 new proposals. Similar to the symposium in 2003 the new proposals were described in oral presentations of 10 minutes each (including discussion). A selection of the renewal proposals was presented in talks of 35 minutes (plus 10 minutes discussion) or 20 minutes (plus 5 minutes discussion). In addition, on the last day four scientists external to the SPP 1145 contributed with lectures. A total of 26 projects (among them 2 joint proposals) were selected for the second financing period of the SPP 1145.

6.1.4 Symposium 2006 (June 26 - 28, 2006, Bad Herrenalb)

Organizer:

- Prof. Dr. Hans-Joachim Werner (Stuttgart), Prof. Dr. Jürgen Gauss (Mainz)

Number of participants: 70

6.1.5 Symposium and review panel meeting 2007 (July 4 - 6, 2005, Bonn)

Organizer:

- Prof. Dr. Michael Dolg (Köln)

Number of participants: 76 (status June 28, 2007)

26 project proposals (among them 2 joint proposals) will be presented on posters, 22 being renewal proposals and 4 new proposals. The new proposals will be described in short oral presentations of 15 minutes (plus 5 minutes discussion). A selection of the renewal proposals will be presented in talks of 30 minutes (plus 5 minutes discussion) or 15 minutes (plus 5 minutes discussion). Some of the shorter talks will be given by young researchers (i.e. PhD students or postdocs). In addition, on the last day in the final session one presentation of a project not asking for renewal of funding as well one of a young researcher not funded through the SPP 1145 will be given.

6.1.6 Programs and lists of participants of the symposia 2005 - 2007

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,
Tel.: ++49 (0)228/98960, http://www.cjd-bonn.de
Program (version June 30, 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 (chair Willem Klopper)
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 (chair Hubert Ebert)
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 (chair Peter Saalfrank)
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 (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 (chair Martin Albrecht)
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 (chair Eberhard Engel)
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 (chair Andreas Görling)

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 (chair Timo Fleig)

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 (chair Arne Lüchow)

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 (chair Gotthard Seifert)

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).

Organization: Michael Dolg, Rebecca Fondermann, Joachim Friedrich, Michael Hanrath, Alexander Schnurpfeil (all Cologne)

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,
Tel.: ++49 (0)228/98960, http://www.cjd-bonn.de

(version June 21, 2005)

Note: the room reservation in the CJD Bonn is indicated as follows

4-6	Monday July 4 to Wednesday July 6 (2 nights)
5-6	Tuesday July 5 to Wednesday July 6 (1 night)
4-5	Monday July 4 to Tuesday July 5 (1 night)
-	no room reservation required

Participants

1. Albrecht, Martin (Siegen) 4-6
2. Andreev, Oleg (Dresden) 4-6
3. Arbuznikov, Alexei (Würzburg) 4-6
4. Birkenheuer, Uwe (Dresden) 4-6
5. Bihlmayer, Gustav (Jülich) -
6. Burkatzki, Mark (Köln) -
7. Chinnamsetty, Sambasiva (Leipzig) 4-6
8. Dolg, Michael (Köln) 4-6
9. Ebert, Hubert (München) 4-6
10. Engel, Eberhard (Frankfurt) 4-6
11. Eschrig, Helmut (Dresden) 5-6
12. Filippi, Claudia (Leiden) 4-6
13. Flad, Heinz-Jürgen (Leipzig) 4-6
14. Fleig, Timo (Düsseldorf) 4-6
15. Fliegl, Heike (Karlsruhe) 4-6
16. Fondermann, Rebecca (Köln) -
17. Fricke, Burkhard (Kassel) 4-6
18. Friedrich, Christoph (Jülich) 4-6
19. Friedrich, Joachim (Köln) -
20. Fritzsche, Stephan (Kassel) 4-6
21. Gaigalas, Gedimas (Kassel) 4-6
22. Gauss, Jürgen (Mainz) 4-6

23. Görling, Andreas (Erlangen) 4-6
24. Goll, Erich (Stuttgart) 4-6
25. Griebel, Michael (Bonn) -
26. Gross, Eberhard (Berlin) 4-6
27. Hättig, Christof (Karlsruhe) 4-6
28. Hamaekers, Jan (Bonn) -
29. Hanrath, Michael (Köln) -
30. Heckert, Miriam (Mainz) 4-6
31. Jansen, Georg (Essen) 4-6
32. Jiang, Hong (Frankfurt) 4-6
33. Kaupp, Martin (Würzburg) 4-6
34. Klopper, Wim (Karlsruhe) 4-6
35. Ködderitzsch, Diemo (München) 4-6
36. Kolb, Dietmar (Kassel) 4-6
37. Kordel, Elena (Karlsruhe) 4-6
38. Kurth, Stefan (Berlin) 4-6
39. Lathiotakis, Nektarios (Berlin) 4-6
40. Lüchow, Arne (Aachen) 4-6
41. Luo, Hongjun (Kassel) 4-6
42. Mata, Ricardo (Stuttgart) 4-6
43. Michauk, Christiane (Mainz) 4-6
44. Moritz, Gerrit (Jena) -
45. Neiss, Christian (Karlsruhe) 4-6
46. Nest, Mathias (Potsdam) 4-6
47. Ochsenfeld, Christian (Tübingen) 4-6
48. Paulus, Beate (Dresden) 4-6
49. Pittalis, Stefano (Berlin) 4-6
50. Plunien, Günter (Dresden) 4-6
51. Rangaswamy, Geethalakshmi (Siegen) 4-6
52. Reiher, Markus (Jena) -
53. Richter, Manuel (Dresden) 4-5
54. Saalfrank, Peter (Potsdam) 4-6
55. Saenz, Alejandro (Berlin) 4-6
56. Saue, Trond (Strasbourg) 4-6
57. Savin, Andreas (Paris) 4-6
58. Schäffer, Rainer (Essen) 4-6
59. Schindlmayr, Arno (Jülich) 4-6
60. Schneider, Reinhold (Kiel) 5-6
61. Schnurpfeil, Alexander (Siegen, Köln) -
62. Schütz, Martin (Regensburg) 4-6
63. Schwinger, Stefan (Leipzig) 4-6
64. Scott, Tony (Aachen) 4-6

65. Sebastiani, Daniel (Mainz) 4-6
66. Seifert, Gotthard (Dresden) 4-6
67. Soerensen, Lasse (Düsseldorf) 4-6
68. Springborg, Michael (Saarbrücken) 4-6
69. Stoll, Hermann (Stuttgart) 4-6
70. Usvyat, Dennis (Würzburg) 4-6
71. Van Wüllen, Christoph (Berlin) 4-6
72. Villani, Christian (Karlsruhe) 4-6
73. Voloshina, Elena (Dresden) 4-6
74. Volotka, Andrei (Dresden) 4-6
75. Weber, Toralf (Kiel) 4-6
76. Werner, Hans-Joachim (Stuttgart) 4-6
77. Wildenhues, Ralf (Bonn) -
78. Wolf, Alexander (Jena) 4-5

Review Panel Board

1. Blöchl, Peter (Clausthal-Zellerfeld) 4-6
2. Domcke, Wolfgang (München) 4-6
3. Gill, Peter (Canberra, Australien) 4-6
4. Goedecker, Stefan (Basel, Schweiz) 4-6
5. Joergensen, Poul (Aarhus, Dänemark) 4-6
6. Lichtenstein, Alexander (Hamburg) 4-6
7. Marx, Dominik (Bochum) 4-6
8. Nieminen, Risto (Espoo, Finnland), will not participate
9. Ordejon, Pablo (Barcelona, Spanien) 4-6
10. Sauer, Joachim (Berlin) 4-6
11. Siedentop, Heinz (München) 4-6
12. Wunner, Günther (Stuttgart) 4-6

DFG

1. Kuchta, Frank-Dieter (Bonn) 4-6

DFG Priority Program SPP 1145

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

Symposium 2006

26 June 2006 – 28 June 2006

Haus der Kirche – Evangelische Akademie Baden
Bad Herrenalb

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

Symposium Bad Herrenalb 2006

List of participants

	Name	Vorname	Titel
1	Adler	Thomas	Dipl. Chem.
2	*Blügel	Stefan	Prof. Dr.
3	Chinnamsetty	Sambasiva Rao	
4	Doser	Bernd	Dipl. Chem.
5	Ebert	Hubert	Prof.
6	Eckard	Simon	Dipl. Chem.
7	*Engel	Eberhard	Dr.
8	Ermrich	Regina	
9	Exner	Thomas E.	Prof. Dr.
10	Flad	Heinz-Jürgen	Dr.
11	Fondermann	Rebecca	
12	Friedrich	Christoph	Dr.
13	Gaston	Nicola	Dr.
14	*Gauss	Jürgen	Prof.
15	Goll	Erich	Dipl. Chem.
16	*Görling	Andreas	Prof. Dr.
17	Götz	Andreas	Dr
18	Gill	Peter	Prof.
19	Hamaekers	Jan	
20	Hanrath	Michael	Dr.
21	Harding	Michael	
22	Heckert	Miriam	
23	Jiang	Hong	Dr.
24	*Klopper	Wim	Prof. Dr.
25	Knizia	Gerald	
26	Ködderitzsch	Diemo	Dr.
27	Kordel	Elena	
28	Kurth	Stefan	Dr.
29	*Kutzelnigg	Werner	Prof.
30	Lambrecht	Daniel	Dipl. Chem.
31	Lathiotakis	Nektarios	Dr
32	Lüchow	Arne	Prof. Dr.
33	Mata	Ricardo	Dipl. Chem.
34	Metzroth	Thorsten	
35	Moritz	Gerrit	
36	Neiß	Christian	Dr.
37	Nest	Mathias	Dr.
38	Paulus	Beate	Dr.
39	Pflüger	Klaus	
40	Pittalis	Stefano	
41	Reiher	Markus	Prof. Dr.
42	Sargolzaei	Mahdi	
43	Schindlmayr	Arno	Dr.
44	Schütz	Martin	Prof. Dr.
45	Scott	Tony	Dr.
46	Siedentop	Heinz	Prof.
47	Simon	Anja	
48	Soerensen	Lasse Kragh	
49	Springborg	Michael	Prof. Dr.
50	*Stoll	Hermann	Prof. Dr.
51	Taut	Manfred	Dr. habil.
52	Tevekeliyska	Violina	Dipl. Chem.
53	Usvyat	Denis	Dr.
54	Voloshina	Elena	Dr.
55	*Werner	Hans-Joachim	Prof. Dr.
56	Wildenhues	Ralf	

Invited external speakers (8)		
*Burke	Kieron	Prof.
Furche	Filipp	Dr.
*Head-Gordon	Martin P.	Prof.
*Harrison	Robert J.	Dr.
*Kresse	Georg	Dr.
*Manby	Fred	Dr.
*Nooijen	Marcel	Prof.
*Pulay	Peter	Prof.

Speakers from the SPP (6)		
Birkenheuer	Uwe	Dr.
*Dolg	Michael	Prof. Dr.
Fleig	Timo	Priv.Doz. Dr.
Hättig	Christof	Prof. Dr.
*Ochsenfeld	Christian	Prof. Dr.
*van Wüllen	Christoph	Prof.

Fifth Meeting of the DFG Priority Program 1145

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

July 4-6, 2007

CJD Bonn, Graurheindorfer Str. 149, D-53117 Bonn,
Tel.: ++49 (0)228/98960, http://www.cjd-bonn.de
Program (version June 6, 2007)

Wednesday, July 4, 2007

until 18:00	**Arrival**
	Project Applicants: Please put posters on display !
18:00 - 19:30	**Dinner** (buffet with self-service for those who arrive late)

Poster session I

19:30 - 22:00	Discussion of the project applicants with the members of the review panel board at the posters

Thursday July 5, 2007

7:00 - 9:00	**Breakfast**
8:30 - 9:00	**Review Panel Board:** First meeting (with Frank-Dieter Kuchta, DFG)
9:00 - 9:15	Welcome (Kuchta, DFG; Dolg, Cologne)

Oral presentations I
(chair: Hans-Joachim Werner (Stuttgart))

9:15 - 9:45	Willem M. Klopper (Karlsruhe) *Recent progress in R12 coupled-cluster theory*
9:45 - 9:50	Discussion
9:50 - 10:05*	Alexander A. Auer (Chemnitz) *New local approaches between conventional and linear scaling coupled cluster methods*
10:05 - 10:10	Discussion
10:10 - 10:25**	Thomas Adler (Stuttgart) *Explicitly correlated local MP2-theory: towards the basis set limit of large molecules*
10:25 - 10:30	Discussion
10:30 - 11:00	**Coffee break and Posters**

Oral presentations II
(chair: Eberhard Gross (Berlin))

11:00 - 11:30	Andreas Görling (Erlangen) *Exact treatment of exchange in density-functional methods*
11:30 - 11:35	Discussion
11:35 - 11:50*	Peter Blöchl (Clausthal-Zellerfeld) *Local correlations in density functional theory using a mixed density and density matrix functional theory*
11:50 - 11:55	Discussion
11:55 - 12:10	Thomas Exner (Konstanz) *Improvements of a fragment-based quantum chemical approach: the border-region problem*
12:10 - 12:15	Discussion
12:15 - 13:30	**Lunch**

Oral presentations III
(chair: Eberhard Engel (Frankfurt))

13:30 - 14:00	Hubert Ebert (München) *Relativistic treatment of spin-polarized atomic and solid state systems*
14:00 - 14:05	Discussion
14:05 - 14:20*	Andreas Dreuw (Frankfurt) *Charge-transfer excited states in time-dependent density functional theory*
14:20 - 14:25	Discussion
14:25 - 14:40**	Joachim Friedrich (Köln) *Fully automatized implementation of the incremental scheme*
14:40 - 14:45	Discussion
14:45 - 15:15	**Coffee break and Posters**

Oral presentations IV
(chair: Helmut Eschrig (Dresden))

15:15 - 15:45	Gotthard Seifert (Dresden) *Non-collinear orbital magnetism in nanostructures and solids*
15:45 - 15:50	Discussion
15:50 - 16:05*	Martin Kaupp (Würzburg) *New occupied-orbital dependent exchange-correlation functionals*
16:05 - 16:10	Discussion

Poster session II

16:30 - 18:00	Discussion of the project applicants with the members of the review panel board at the posters
18:00 - 19:30	**Dinner*****
18:00 - ..:..	**Review panel board:** Second meeting (including dinner)

Friday July 6, 2007

7:00 - 8:30	**Breakfast**
	Oral presentations V
	(chair: Michael Griebel (Bonn))
8:30 - 9:00	Michael Springborg (Saarbrücken)
	Infinite, periodic systems in external electrostatic fields
9:00 - 9:05	Discussion
9:05 - 9:20	Beate Paulus (Dresden)
	The method of increments for metals
9:20 - 9:25	Discussion
9:25 - 9:40**	Jan Hamaekers (Bonn)
	Sparse grid methods for the electronic Schrödinger equation
9:40 - 9.45	Discussion
9:45 - 10:15	**Coffee break**
10:00 - 16:00	**Review panel board:** Third meeting (including lunch)
	Oral presentations VI
	(chair: Peter Saalfrank (Potsdam))
10:15 - 10:45	Arne Lüchow (Aachen)
	Nodal hypersurfaces of molecular wave functions and quantum Monte Carlo
10:45 - 10:50	Discussion
10:50 - 11:20	Hermann Stoll (Stuttgart)
	Explicit treatment of long-range exchange-correlation in denisty functional theory
11:20 - 11:25	Discussion
11:25 - 11:55**	Darragh O'Neill (Mainz)
	Hyperpolarizabilities, Raman intensities and anharmonic force constants: steps towards analytic third derivatives in coupled-cluster theory
11:55 - 12:00	Discussion
12:00 - 14:00	**Lunch*****
	Departure

* presentation of a proposal for a new project in the priority program.

** presentation by a young researcher.

*** lunch/dinner for the review panel board members will be served separately.

Organization: Michael Dolg, Rebecca Fondermann, Joachim Friedrich, Michael Hanrath
Anna Moritz, Jonas Wiebke

Fifth Meeting of the DFG Priority Program 1145

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

July 4-6, 2007

CJD Bonn, Graurheindorfer Str. 149, D-53117 Bonn,
Tel.: ++49 (0)228/98960, http://www.cjd-bonn.de

(version June 28, 2007)

Participants

Adler, Thomas (Stuttgart)
Arbuznikov, A. V. (Würzburg)
Auer, Alexander (Chemnitz)
Berner, Raphael (Aachen)
Bihlmayer, Gustav (Jülich)
Blauert, Johannes (Kiel)
Blöchl, Peter (Clausthal-Zellerfeld)
Blügel, Stefan (Jülich)
Burkatzki, Mark (Köln)
Chadov, Stanislav (München)
Chaplygine, Igor (Dresden)
Dolg, Michael (Köln)
Dong, Yi (Saarbrücken)
Doser, Bernd (Tübingen)
Dreuw, Andreas (Frankfurt)
Ebert, Hubert (München)
Eckard, Simon (Konstanz)
Engel, Eberhard (Frankfurt)
Eschrig, Helmut (Dresden)
Exner, Thomas (Konstanz)
Flad, Heinz-Jürgen (Kiel)
Fleig, Timo (Düsseldorf)
Fondermann, Rebecca (Köln)
Fox-Beyer, Brigitte (Berlin)
Friedrich, Joachim (Köln)
Görling, Andreas (Erlangen)
Griebel, Michael (Bonn)
Gross, Eberhard (Berlin)

Hackbusch, Wolfgang (Leipzig)
Hättig, Christoph (Bochum)
Hamaekers, Jan (Bonn)
Hanrath, Michael (Köln)
Ipatov, Andrej (Erlangen)
Kats, Danylo (Regensburg)
Kaupp, Martin (Würzburg)
Klopper, Wim (Karlsruhe)
Knizia, Gerald (Stuttgart)
Ködderitzsch, Diemo (München)
Kordel, Elena (Karlsruhe)
Kurth, Stefan (Berlin)
Lambrecht, Daniel (Tübingen)
Lüchow, Arne (Aachen)
Metzroth, Thorsten (Mainz)
Moritz, Anna (Köln)
Neise, Carsten (Dresden)
Nest, Mathias (Potsdam)
Ochsenfeld, Christian (Tübingen)
O'Neill, Darragh (Mainz)
Paulus, Beate (Dresden)
Pittalis, Stefano (Berlin)
Rao, Sambasiva (Kiel)
Richter, Manuel (Dresden)
Rohwedder, Thorsten (Kiel)
Saalfrank, Peter (Potsdam)
Schindlmayr, Arno (Jülich)
Schneider, Reinhold (Kiel)
Schütz, Martin (Regensburg)
Seifert, Gotthard (Dresden)
Sorensen, Lasse Kragh (Düsseldorf)
Springborg, Michael (Saarbrücken)
Stoll, Hermann (Stuttgart)
Taut, Manfred (Dresden)
Tevekeliska, Violina (Saarbrücken)
van Wüllen, Christoph (Berlin)
Voloshina, Elena (Dresden)
Walther, Christian (Clausthal-Zellerfeld)
Werner, Hans-Joachim (Stuttgart)
Wiebke, Jonas (Köln)
Yang, Jun (Bochum)

Review Panel Board

Gill, Peter (Canberra)
Goedecker, Stefan (Basel)
Lichtenstein, Alexander (Hamburg)
Marx, Dominik (Bochum)
Sauer, Joachim (Berlin)
Siedentop, Heinz (München)
Szalay, Peter (Budapest)
Valenti, Maria-Roser (Frankfurt)

DFG

Kuchta, Frank-Dieter (Bonn)

6.2 Workshops

In the second financing period two workshops were organized within the SPP 1145 in 2006 and 2007, cf. the programmes and listings of participants given below.

During the third financing period several workshops are under consideration. A workshop focussing on coupled-cluster methods is planned by Alexander Auer (Chemnitz), Michael Hanrath (Cologne), and Christan Ochsenfeld (Tübingen) for 2009. Another workshop organized by Peter Saalfrank (Potsdam) is under discussion.

6.2.1 Workshop *First-principles approaches to optical and photoelectron spectra* (March 11 - 13, 2005, Berlin)

Organizers:

- Prof. Dr. Claudia Ambrosch-Draxl (Graz)
- Prof. Dr. Eberhard K. U. Gross (Berlin)
- Prof. Dr. Hubert Ebert (München)
- Prof. Elisa Molinari (Modena)

Number of participants: 50

homepage: http://olymp.cup.uni-muenchen.de/ak/ebert/FOPS06

The Munich group (Hubert Ebert, LMU) involved in the SPP 1145 together with Eberhard K. U. Gross (Freie Universität Berlin, also member of the SPP 1145), Claudia Ambrosch-Draxl (Universität Graz) and Elisa Molinari (University of Modena and Reggio Emilia) organized an international workshop entitled *First-principles approaches to optical and photoelectron spectra*, 9-12 March 2006 in Munich, that attracted more than 50 participants. A central issue of all contributions was the impact of correlation effects on spectroscopic properties. It was centered around theoretical approaches and encompassed a broad range of methods, e.g. *GW* and beyond, exact exchange methods and Dynamical Mean Field Theory.

6.2.2 Workshop *Highly accurate calculations of molecular electronic structure* (March 22 - 24, 2007, Bad Herrenalb

Organizers:

- Prof. Dr. Willem Marten Klopper (Karlsruhe)

Number of participants: 87

homepage: http://www.ipc.uni-karlsruhe.de/tch/spp1145

6.2.3 Programs and lists of participants of workshops 2006 - 2007

First-principles approaches to optical and photoelectron spectra

Organizers
Participants
Program
Abstracts
Talks
Conference site/ How to arrive
Conference fee
Accomodation

Workshop

9-12 March 2006

LMU Munich

Email : Michal.Kosuth@cup.uni-muenchen.de

This workshop is financed by Deutsche Forschungsgemeinschaft DFG

within the priority program Modern and universal first-principles methods for many electron systems in chemistry and physics

and the EU-funded network EXCiTiNG

Last changes: Feb 15, 2006

2 Program

Thursday, 17.30 – 19.00 Registration

Time	Friday	Saturday	Sunday
9.00 – 9.40	**Di Felice** Electronic structure of DNA-based derivatives and mimics by DFT	**Chulkov** Electron and hole dynamics in bulk metals and at surfaces	**Shaltaf** First Principle Calculations Of Different Material Band Offsets With Silicon
9.40 – 10.00	**Ernst** Multiple-scattering concept of a real-space GW approximation	**Henk** Photoelectron spectroscopy of spin-orbit split surface states	**Chaplygin** LDA+U and Hund's second rule
10.00 – 10.20			Coffee Break
10.20 – 10.30	**Floris** Gap anisotropy in density functional theory of the superconducting state	**Braun** Relativistic photoemission theory for correlated systems	
10.30 – 10.40			**Hohenester** Optical near-field mapping of bright and dark quantum dot states
10.40 – 11.10	Coffee Break	Coffee Break	
11.10 – 11.30	**Pavlyuk** GW approximation for finite systems	**Aeschlimann** Lifetimes of quasiparticle excitations in metals and organic semiconductors	**Plasencia** Lifetime of electrons in the excited states of quantum dots
11.30 – 11.50			
11.50 – 12.30	**Reining** Beyond the GW approximation	**Schattke** Aspects of high photon intensity in ARPES	Departure
12.30 – 12.50	**Nekrasov** Computation of pseudogap regime for underdoped Bi2212 within LDA+DMFT+ $\Sigma_{\mathbf{k}}$ approach	**Krasovskii** Elastic and Inelastic Scattering in Photoemission: a Band Structure Theory	
11.50 – 12.30	Lunch	Lunch	

14.20 - 15.00	**Panaccione** Surface vs. bulk electronic properties of strongly correlated system	**Gunnarson** Interplay between Coulomb and electron-phonon interactions in cuprates	
15.00 – 15.40	**Potthoff** A variational approach to photoemission spectra for strongly correlated electron systems	**Lindroos** Lindroos Angle resolved photoemission from high-t_c cuprates	
15.40 – 16.00	**Helbig** Orbital Functionals in Current Spin Density Functional Theory	**Saha** Optical properties of random alloys	
16.00 – 16.30	Coffee Break	Coffee Break	
16.30 – 17.10	**Sharma** Optimized Effective Potential Method for Non-Collinear Magnetism	**Puschnig** Excitons in organic semiconductors	
17.10 – 17.30	**Lathiotakis** Reduced Density Matrix Functional Theory for the homogeneous electron gas	**Rohlfing** Structural relaxations in electronically excited poly-para-phenylene	
18.00 – 19.30	Poster Session	EXCITING network meeting	
19.30 –		Dinner	

3 Participants

Invited Speakers

- M. Aeschlimann, Kaiserslautern, Germany
- E. Chulkov, San Sebastian, Spain
- R. Di Felice, Modena, Italy
- A. Ernst, Halle, Germany
- O. Gunnarson, Stuttgart, Germany
- J. Henk, Halle, Germany
- U. Hohenester, Graz, Austria
- J. Inglesfield, Cardiff, England
- W. Ku, Brookhaven National Laboratory, USA
- R. Laskowski, Aarhus, Denmark
- M. Lindroos, Tampere, Finnland
- G. Panaccione, Trieste, Italy
- Y. Pavlyukh, Kaiserslautern, Germany
- M. Potthoff, Würzburg, Germany
- P. Puschnig, Montanuniversität Leoben, Austria
- L. Reining, Paris, France
- W. Schattke, Kiel, Germany
- R. Shaltaf Louvain la Neuve, Belgium
- S. Sharma, FU Berlin, Germany/ KFU Graz, Austria

Speakers - contributed talks

- J. Braun, LMU Munich, Germany
- I. Chaplygin, TU Dresden, Germany
- A. Floris, FU Berlin, Germany
- N. Helbig, FU Berlin, Germany
- E. Krasovskii, CAU Kiel, Germany
- N. Lathiotakis, FU Berlin, Germany
- I. Nekrasov, Ekaterinburg, Russia
- M. Rohlfing, Osnabrueck, Germany
- C. Plasencia, Modena, Italy
- S. Sagmeister, Uni Graz, Austria
- K. Saha, MPI Halle, Germany

Participants

- S. Bornemann, LMU Munich, Germany
- S. Chadov, LMU Munich, Germany
- R. Fortrie, HU Berlin, Germany
- S. Goumri-Said, Kaiserslautern, Germany

- R. Hott, IFP Karlsruhe, Germany
- J.-O. Joswig, Helsinki, Finland
- M. Kosuth, LMU Munich, Germany
- D. Ködderitzsch, LMU Munich, Germany
- S. Kurth, FU Berlin, Germany
- S. Mankovsky, LMU Munich, Germany
- L. Martin-Samos, Modena, Italy
- J. Minar, LMU Munich, Germany
- W. Olovsson, Kyoto, Japan
- S. Polesya, LMU Munich, Germany
- M. Rapacioli, TU Dresden, Germany
- G. Stefanucci, FU Berlin, Germany
- L. Tunturivuori, Helsinki, Finland
- M. Walter, Jyväskylä, Finland
- J. Werschnik, FU Berlin, Germany
- W. Wunderlich, Nagoya, Japan
- A. Zacarias, FU Berlin, Germany

4 Talks

- Rosa Di Felice

  Electronic structure of DNA-based derivatives and mimics by DFT

  National Center S3 of INFM-CNR,Via Campi 213/A, 41100 Modena, Italy

- Arthur Ernst

  Multiple-scattering concept of a real-space GW approximation

  Max-Planck-Institut für Mikrostrukturphysik Halle(Saale), 06120, Germany

- Andrea Floris

  Gap anisotropy in density functional theory of the superconducting state

  Freie Universitaet Berlin,Theoretische Physik Arnimallee 14D-14195 Berlin

- Yaroslav Pavlyukh

  GW approximation for finite systems

  Technical University of Kaiserslautern,FB Physik, TU Kaiserslautern, Erwin-Schrödinger-Str. 46, D-67663 Kaiserslautern

- Lucia Reining

  Beyond the GW approximation

  LSI CNRS/CEA/Ecole Polytechnique,Ecole Polytechnique, 91128 Palaiseau, France

- Igor Nekrasov

  Computation of pseudogap regime for underdoped Bi2212 within LDA+DMFT+Σ_k approach.

  Institute of Electophysics Ural Branch of Russian Academy of Sciences,620016, Russia, Ekaterinburg, Amundsena Str. 106

- Giancarlo Panaccione

  Surface vs. bulk electronic properties of strongly correlated system

  Lab. TASC - INFM -CNR,Area Science Park Basovizza (trieste) Italy

- Michael Potthoff

  A variational approach to photoemission spectra for strongly correlated electron systems

  Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, 97074 Würzburg

- Wolfgang Schattke

  Aspects of high photon intensity in ARPES

  Institut für Theoretische Physik und Astrophysik der Christian-Albrechts-Universität zu Kiel and Donostia International Physics Center (DIPC),Leibnizstr. 15, D-24118 Kiel, Germany

- Eugene Krasovskii

  Elastic and Inelastic Scattering in Photoemission: a Band Structure Theory

  Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität,Leibnizstr. 15, 24118 Kiel, Germany

- Matti Lindroos

  Angle resolved photoemission from high-t_c cuprates

  Tampere University of Technology,P.O. Box 692, Tampere, Finnland

- Kamal Saha

  Optical properties of random alloys

  Max-Planck-Institut für Mikrostrukturphysik,Weinberg 2, D-06120 Halle (Saale), Germany

- Peter Puschnig

  Excitons in organic semiconductors

  Chair of Atomistic Modeling and Design of Materials, Montanuniversität Leoben,Erzherzog-Johannstraße 3, A-8700 Leoben, Austria

- Michael Rohlfing

  Structural relaxations in electronically excited poly-para-phenylene

  Universitaet Osnabrueck,Barbarastrasse 7, 49069 Osnabrueck, Germany

- Riad Shaltaf

  First Principle Calculations Of Different Material Band Offsets With Silicon

  Université catholique de Louvain, Unité Physico-Chimie et de Physique des Matériaux (PCPM), Université catholique de Louvain, Place Croix du Sud, 1 B-1348, Louvain-la-Neuve Belgique

- Igor Chaplygin

  LDA+U and Hund's second rule

  TU Dresden, Institut für Physikalische Chemie und Elektrochemie, 01062 Dresden

- Ulrich Hohenester

  Optical near-field mapping of bright and dark quantum dot states

  Univ. Graz, Inst. für Physik, Universitätsplatz 5, 8010 Graz, Austria

- Juan Ignacio Climente Plasencia

  Lifetime of electrons in the excited states of quantum dots

  CNR-INFM S3,Via Campi 213/A, 41100, Modena, Italy

5 Posters

- Stanislav Chadov

  Magneto-optical properties of systems with local electronic correlations

  Department Chemie und Biochemie, Physikalische Chemie, Universität München, Butenandtstr. 5-13, D-81377 München, Germany

- Remy Fortrie

  Two-photo absorption strength: A new tool for the quantification of two-photon absorption

  Institut fuer Chemie, Humboldt-Universitaet zu Berlin, Unter den Linden 6, 10099 Berlin

- Souraya Goumri-Said

  First principles calculations of electronic and magnetic properties of Co_5 cluster

  Condensed Matter Group. Department of Physics,Kaiserslautern University of Technology , Erwin-Schrdinger strae 46, Box 3049. D-67653 Kaiserslautern. Germany

- Mohammed-Benali Kanoun

  Electronic structure and magnetism of Eu-doped GaN: A first-principles study

  Institut dElectronique de Microélectronique et de Nanotechnologie UMR CNRS 8520, Université de Sciences et Technologie de Lille., Avenue Poincaré, BP 60069, 59652 Villeneuve dAscq Cedex, France

- Diemo Ködderitzsch

  A relativistic optimised potential method for spin-polarised systems – application to alkali and transition metals

  Ludwig-Maximilians-Universität München, Department Chemie, Physikalische Chemie, Germany

- Stefan Kurth

  A Practical Scheme for Quantum Transport with Applications to Electron Pumping

  Institute for Theoretical Physics, Free University Berlin, Arnimallee 14, 14195 Berlin

- Franca Manghi

  Theoretical Simulation of Many Body Effects in Photoemission Spectra

  University of Modena - S3, via Campi 213, Modena Italy

- Layla Martin-Samos

  The SaX project, implementation of a GW-BSE code

  CNR-INFM-S3,via Campi 213, Modena, Italy

- Jan Minar

  Multiple scattering formalism for correlated systems: A KKR+DMFT approach

  Dep. Chemie und Biochemie, Physikalische Chemie, Universität München, Butenandtstr. 5-13, D-81377 München, Germany

- Mathias Rapacioli

  Electronic spectroscopy of interstellar PAH clusters

  TU Dresden, TU Dresden, Institut fr Physikalische Chemie und Elektrochemie, Erich-Mller-Bau, Bergstrae 66b, 01062 Dresden

- Stephan Sagmeister

  Time-dependent density functional theory within an all electron framework

  Institute for Physics / Theoretical Physics,Universitaetsplatz 5, A-8010 Graz

- Reinhard Scholz[1], Igor Vragovic[2] and Linus Gisslen[3]

  Spectroscopic properties of molecular crystals composed of perylene-based chromophores

  [1] *Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, D-85748 Garching*
  [2] *Departamento de Fisica Aplicada, Universidad de Alicante, E-03080 Alicante, Spain*
  [3] *Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany*

- Gianluca Stefanucci

  Classical nuclear motion in quantum transport

  Institute for Theoretical Physics, Free University Berlin, Arnimallee 14, 14195 Berlin, Germany

- Lasse Tunturivuori and Jan-Ole Joswig

  Comparison of approximations to the exchange-correlation functional in the calculation of the dipole-oscillator strength

  Laboratory of Physics, Helsinki University of Technology, P. O. Box 1100, 02015 HUT, Finland

- Michael Walter

  Photoionisation using Kohn-Sham wave functions

  University of Jyväskylä,PL 35 (YFL), Finland

- Jan Werschnik

  Optimal control of electron dynamics using TDDFT

  Freie Universitaet Berlin,Arnimallee 14; 14195 Berlin

- Wilfried Wunderlich

  Ab-initio calculations of the Effective Electron Mass and of SrTiO3 based Thermoelectric Nano-Materials

  Nagoya Instituite of Technology,Dept. Eng. Ohsato-Lab, 466-8555 Nagoya, Japan

SPP 1145 Workshop

Highly Accurate Calculations of Molecular Electronic Structure

Bad Herrenalb, 22–24 March 2007

A workshop of the DFG Priority Program 1145 on "Modern and universal first-principles methods for many-electron systems in chemistry and physics".

Contact
Email: klopper@ipc.uka.de
Tel.: +49(0) 721 608 7263
Fax: +49(0) 721 608 3319

Photograph by Tourismusbüro Bad Herrenalb

The workshop will focus on highly accurate calculations using wavefunction-based methods. Topics include basis-set design and convergence, explicitly-correlated wavefunctions, multireference approaches, high-level coupled-cluster methods, alternative methods (e.g. Monte Carlo), and so on.

Confirmed Speakers

H.-J. Flad (MPI-MIS, Leipzig)
J. Gauß (Mainz)
M. Hanrath (Cologne)
M. Kállay (TU Budapest)
H. Koch (NTNU Trondheim)
A. Köhn (Mainz)
J. Komasa (Poznan)
A. Lüchow (RWTH Aachen)
J. M. L. Martin (Weizmann Inst., Rehovot)
J. Noga (Bratislava)
J. Olsen (Århus)
B. Paulus (MPI-PKS, Dresden)
K. A. Peterson (Washington State U)
M. Schütz (Regensburg)
J.F. Stanton (U of Texas, Austin)
P.G. Szalay (Eötvös U Budapest)
S. Ten-no (Nagoya)
E.F. Valeev (Georgia Inst. of Tech.)
H.-J. Werner (Stuttgart)

Organizer W. Klopper, Universität Karlsruhe (TH), D-76128 Karlsruhe, Germany.
Deadlines Registration: 12 January 2007. Abstract submittal: 9 February 2007.
Conference fee € 150,00 (including accommodation with full board).

Registration forms are available from the conference web site:

http://www.ipc.uni-karlsruhe.de/tch/spp1145

Thursday, 22 March 2007

13:00	Arrival	
13:00–14:30	Lunch	
14:40–14:45	Welcome: W. Klopper	
	Chair: C. Ochsenfeld	
14:45–15:25	**L 1**	**M. Schütz** Local Correlation Methods for Excited States and Periodic Systems
15:25–16:05	**L 2**	**B. Paulus** Quantum Chemical Correlation Treatment for Metals: The Method of Increments Applied to Group II Metals
16:05–16:40	Coffee break	
	Chair: W. Hackbusch	
16:40–17:20	**L 3**	**H.-J. Flad** Tensor Product Approximation in Quantum Chemistry
17:20–18:00	**L 4**	**H. Koch** Method Specific Cholesky Decomposition: Coulomb and Exchange energies
18:00–20:00	Dinner	
20:00–23:00	Poster session	

Friday, 23 March 2007

	Chair: R. F. Fink	
09:00–09:40	**L 5**	**M. Hanrath** Multi-reference Coupled Cluster: Fundamentals, Difficulties and Recent Advances
09:40–10:20	**L 6**	**J. Olsen** Bridging the Gap between Multi-reference Perturbation and Coupled Cluster Methods
10:20–11:00	**L 7**	**S. Ten-no** A Simple F12 Correction in Multi-reference Perturbation Theory
11:00–11:35	Coffee break	
	Chair: C. Puzzarini	
11:35–12:15	**L 8**	**J. Gauss** High-Accuracy Prediction of Molecular Equilibrium Geometries
12:15–12:55	**L 9**	**M. Kállay** High-Accuracy Calculation of Molecular Response Properties
13:00–14:30	Lunch	
	Chair: F. Jensen	
14:30–15:10	**L 10**	**J. F. Stanton** The HEAT Family of Thermochemical Methods: Results and Underlying Theoretical Advances
15:10–15:50	**L 11**	**J. M. L. Martin** Basis Set Convergence of Post-CCSD(T) Correlation Contributions. W4 Theory: Confident Sub-kJ/mol Accuracy Computational Thermochemistry
15:50–16:25	Coffee break	
	Chair: P. R. Taylor	
16:25–17:05	**L 12**	**J. Noga** Different Considerations for Second Order R12/F12 Theory
17:05–17:45	**L 13**	**H.-J. Werner** Recent Advances in Explicitly Correlated Local Correlation Methods
17:45–18:25	**L 14**	**K. A. Peterson** Correlation Consistent Basis Sets for Explicitly Correlated MP2-F12 Calculations
18:30–20:30	Dinner	

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Chair: F. R. Manby

09:00–09:40 **L 15 J. Komasa**
The Method of Exponentionally Correlated Gaussian Wave Functions: An Overview, Implementation, Performance and Perspectives

09:40–10:20 **L 16 A. Lüchow**
Quantum Monte Carlo: Recent Developments

10:20–11:00 **L 17 E. F. Valeev**
Explicitly Correlated R12 Methods For Thermochemistry

11:00–11:35 Coffee break

Chair: M. Dolg

11:35–12:15 **L 18 A. Köhn**
Behaviour of Non-Hermitian Methods at Near-Degeneracies

12:15–12:55 **L 19 P. G. Szalay**
Analytic Calculation of the Diagonal Born-Oppenheimer Correction within Coupled-Cluster Theory

13:00–14:30 Lunch

14:30 Departure

Posters

P 1 **T. B. Adler, H.-J. Werner, F. R. Manby**
Linear scaling DF-LMP2-F12 theory

P 2 **J. Aguilera-Iparraguirre, H. J. Curran, W. Klopper, J. M. Simmie**
Calculation of Reaction Rates for Hydrogen Abstraction by the Hydroperoxyl Radical from C1 through C4 Hydrocarbons

P 3 **A. A. Auer**,
Screening in Local Coupled-Cluster Methods - Perspectives for an Efficient Scheme

P 4 **R. A. Bachorz, W. Klopper**
Explicitly correlated study on adiabatic electron affinity and relative stability of various tautomers of anionic uracil

P 5 **P. Dahle, T. Helgaker, D. Jonsson, P. R. Taylor**
Accurate MP2 correlation energies from mixed Gaussian-type orbital and Gaussian-type geminal basis sets

P 6 **B. Doser, D. S. Lambrecht, C. Ochsenfeld**
A Linear-Scaling AO-MP2 Method by Rigorous Integral Screening Criteria

P 7 **R. F. Fink**
Retaining the Excitation Degree Perturbation Theory for Multi Configuration electronic Structure cases. Concept, Performance, Problems, Solutions

P 8 **B. S. Fox-Beyer, C. van Wüllen**
Theoretical Modeling of the Adsorption of Heavy and Superheavy Element Atoms on Gold Surfaces using Two-Component Density Functional Methods with Pseudopotentials

P 9 **J. Franz, A. Takatsuka, S. Ten-no, J. Tennyson**
Calculation of Positron Binding Energies to Molecules using Møller-Plesset Perturbation Theory with Slater-type Geminals

P 10 **J. Friedrich, M. Hanrath, M. Dolg**
Fully Automated Implementation of the Incremental Scheme: Application to CCSD Energies for Carbonhydrides and Transition Metal Compounds

P 11 **E. Goll, H. Stoll, H.-J. Werner**
Short-range DFT/long-range CC methods: new results

P 12 **M. Griebel, J. Hamaekers, R. Wildenhues**
Dimension-adaptive sparse grid methods for the electronic Schrödinger equation

P 13 **M. E. Harding, J. Vázquez, G. Diezemann, J. F. Stanton, J. Gauss**
Vibrational corrections to nuclear magnetic shielding constants computed via a discrete variable representation approach

P 14 **J. G. Hill, J. A. Platts, H.-J. Werner**
Spin-Component Scaling in Intermolecular Interactions

P 15 **F. Jensen**
Polarization Consistent Basis Sets. The Elements He, Li, Be, B, Ne, Na, Mg, Al and Ar

P 16 **A. Karton, J. M. L. Martin**
Heats of Vaporization of Beryllium, Boron, Aluminum, and Silicon Re-Examined by means of W4 Theory

P 17 **D. Kats, T. Korona, M. Schütz**
Transition strength and first-order properties of excited states from local CC2 for large molecules

P 18 **C. G. Knizia, H.-J. Werner**
Orbital invariant explicitly correlated MP2 for high-spin open shell reference states

P 19 **T. Korona**
Exchange-induction interaction energy from one- and two-electron density matrices of monomers

P 20 **A. Kuc, T. Heine, G. Seifert, H. Duarte**
Second order Møller-Plesset treatment of hydrogen physisorption on Metal-Organic Frameworks

P 21 **D. S. Lambrecht, B. Doser, C. Ochsenfeld**
Efficient Strategies for the Linear-Scaling Calculation of Møller-Plesset Correlation Energies

P 22 **O. Lehtonen, D. Sundholm**
Coupled-cluster studies of excited states of oligosilanes

P 23 **Y.-C. Lin, D. Sundholm**
Experimental and Computational Studies of Alkali-Metal Coinage-Metal Clusters

P 24 **F. Manby, C. Woods**
Effective treatment of solvation effects

P 25 **T. Metzroth, M. Kállay, J. Gauss**
Scaling reduced CCSD(T) and CCSDT(Q) methods by decomposition schemes

P 26 **C. Neiss, C. Hättig**
Explicitly-correlated coupled-cluster methods for nonlinear properties: the N_2 molecule

P 27 **D. O'Neill, M. Kállay, J. Gauss**
Dynamic hyperpolarizabilities and Raman intensities calculated within coupled-cluster theory

P 28 **C. Puzzarini, J. Gauss**
Accurate molecular structure calculations for accurately predicting rotational spectra

P 29 **S. Schweizer, M. Kümin, L.-S. Sonntag, H. Wennemers, C. Ochsenfeld**
Quantum Chemical Investigations on the Structure of Substituted Polyproline Systems

P 30 **K. R. Shamasundar, M. Nooijen**
Multi-reference coupled-cluster method using many-body similarity transformed Hamiltonian in diagonalization space including reference and singly excited determinants

P 31 **L. K. Sørensen, T. Fleig, J. Olsen**
Implementation and Initial Application of Multi-Reference Coupled-Cluster

P 32 **C. Sumowski, C. Ochsenfeld**
Accuracies of NMR Chemical Shift Calculations for Large Molecules

P 33 **D. P. Tew, W. Klopper, C. Neiss, C. Hättig**
Quintuple-zeta quality coupled-cluster correlation energies with triple-zeta basis sets

P 34 **D. Usvyat, M. Schütz**
Ground state properties for periodic systems at the LMP2 level

P 35 **J. Vázquez, J. F. Stanton**
High-Order Corrections to the Rotational Constants by Vibrational-Rotational Perturbation Theory

P 36 **E. Voloshina, B. Paulus**
Wavefunction-based ab initio method for metals: application of the incremental scheme to magnesium

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