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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Michael Dolg
Institut für Theoretische Chemie,
Universität zu Köln, Greinstr. 4, D-50939 Köln, Germany

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1 Steering Committee

Prof. Dr. Michael Dolg,
Institut für Physikalische und Theoretische Chemie, Rheinische Friedrich-Wilhelms-Universität Bonn, Wegelerstr. 12, 53115 Bonn,
Tel (0228) 73-3839, Fax (0228) 73-9066,
e-mail dolg@thch.uni-bonn.de

Prof. Dr. Hubert Ebert,
Institut für Physikalische Chemie, Ludwig-Maximilians-Universität München, Butenandtstraße 5–13, 81377 München,
Tel (089) 2180-7583, Fax (089) 2180-7584,
e-mail Hubert.Ebert@cup.uni-muenchen.de

Priv.-Doz. Dr. Eberhard Engel,
Center for Scientific Computing,
Institut für Theoretische Physik, Johann Wolfgang Goethe-Universität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt/Main,
Tel (069) 798-47351, Fax (069) 798-47360,
e-mail engel@th.physik.uni-frankfurt.de

Prof. Dr. Jürgen Gauss,
Institut für Physikalische Chemie, Universität Mainz, Jakob-Welder-Weg 11, 55099 Mainz,
Tel (06131) 392-3736, Fax (06131) 392-3768,
e-mail gauss@slater.chemie.uni-mainz.de

Prof. Dr. Eberhard K. U. Gross,
Institut für Theoretische Physik
Freie Universität Berlin
Arnimallee 14
14195 Berlin
Tel (030) 838-54784, Fax (030) 838-55258
e-mail hardy@physik.fu-berlin.de

Prof. Dr. Hans-Joachim Werner,
Institut für Theoretische Chemie, Universität Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart,
Tel (0711) 685-4401, Fax (0711) 685-4442,
e-mail werner@theochem.uni-stuttgart.de

Prof. Dr. Bernd Artur Heß †
Our colleague and member of the steering committee Prof. Dr. Bernd Artur Heß (Institut für Physikalische und Theoretische Chemie, Universität Bonn) died on July 17, 2004.

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 present report summarizes the development and activities of the SPP 1145 since then until the third symposium and second review panel meeting July 4 - 6, 2005 in Bonn. Some additional information is available on the homepage of the SPP 1145, i.e., http://www.uni-koeln.de/spp1145, as well as on the homepages of the workshops organized within the SPP 1145 (cf. below).

The second symposium of the priority program 1145, without review panel meeting, was held May 24 - 25, 2004 in Bonn (oragnization: B. A. Heß †) and covered nearly all branches of research carried out in the priority program. 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. In addition, 10 new project proposals were made. These numbers show that there is a large interest of research groups in Germany to contribute to new directions in the field of electronic structure theory. All three symposia were/are financed directly by the DFG. Conference programmes as well as lists of participants are given in section 6.1. The 2006 symposium will be probably held in June in Bad Herrenalb (organization: H.-J. Werner, J. Gauss).

In addition to the symposia workshops were organized on specialized topics, i.e., *Numerical Analysis in Quantum Chemistry* (in Kiel; organizers: R. Schneider, W. Hackbusch, B. Hartke) and *Orbital functionals for exchange and correlation* (in Berlin; organizers: S. Kurth, E. K. U. Gross, H. Ebert). SPP 1145 project leaders as well as their coworkers were provided with up to 300,– Euro for enabling their participation for each of the workshops. Besides speakers from the SPP 1145 for all three events, a number of (international) scientists external to the priority program 1145 has also been invited for presentations and was financed or co-financed through the SPP 1145 coordination fonds. 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. Workshop programmes as well as lists of participants are given in section 6.2. At least two additional workshops are planned, i.e., for 2006 on *First-principles approaches to optical and photoelectron spectra* (organizers: H. Ebert, E. K. U. Gross) and for 2007 on *Highly Accurate Molecular Electronic Structure Methods* (organizer: W. Klopper).

At the beginning of the financing period, each project was assigned from the coordination fonds 1.500,– Euro for travel expenses and 1.100,– Euro for financing guests. Due to this financial support many participants of the priority program 1145 were enabled to participate in conferences and workshops external to the SPP 1145 or to visit other research

groups. Many scientists external to the SPP 1145 could be invited for visits to one of the groups being part of the program. A table summarizing these activities is given below in section 6.3.

A total number of 48 publications in international peer-reviewed journals resulted so far from the research carried out within the SPP 1145. An additional 14 manuscripts are currently in press or accepted for publication and further 10 manuscripts have been submitted (status of July 1, 2005). A list of publications is given in section 5. Since the development of new methods often is not a straightforward task and usually takes much more time than pure application work, many more publications are expected in the coming years.

Unfortunately, in the last year we lost two colleagues and project leaders in our priority program due to untimely death. Prof. Dr. Bernd Artur Heß (Bonn), one of the initiators of the present program and a member of the SPP 1145 steering committee, died on July 17, 2004, just a few weeks after he organized the second symposium. Only a few months later Prof. Dr. Gerhard Soff (Dresden) passed away on December 10, 2004. Both were excellent scientists working especially on the field of relativistic and highly correlated ab initio electronic structure methods for heavy element systems. Both leave a gap on their field of science as well as in our SPP 1145 which will be difficult to fill. In order to continue the research and to secure their research assistants working within the SPP 1145, the DFG agreed to hand over the leadership for their projects to their former collaborators Prof. Dr. Markus Reiher (Jena) and Priv.-Doz. Dr. Günther Plunien (Dresden).

Several of the younger current project leaders aquired permanent positions during the last two years. Priv.-Doz. Dr. Eberhard Engel, member of the SPP 1145 steering committee, obtained a permanent position at the Center of Scientific Computing in Frankfurt. In 2004 Martin Schütz was appointed a C3 professorship at the university of Regensburg and Andreas Görling moved from Bonn to a C4 professor position in Erlangen. Markus Reiher accepted an offer to a W2 professor position at the university of Jena in 2005. Recently Christof Hättig received an offer for a W2 professor position at the university of Bochum. These promotions also reflect the high scientific quality of the work, partly carried out within the SPP 1145, of these colleagues.

Finally two members of our program received awards for their excellent scientific work. Prof. Dr. Jürgen Gauss (Mainz), also member of the SPP 1145 steering committee, received the Gottfried Wilhelm Leibniz-Preis 2005 for his outstanding contributions to molecular quantum chemistry. Priv.-Doz. Dr. Christof Hättig (Karlsruhe) was awarded the Hans-Hellmann-Preis of the Arbeitsgemeinschaft Theoretische Chemie in 2004 for his important contributions to coupled-cluster response theory and the treatment of excited states of large molecules using the RI-CC2-approach. Congratulations to all of them !

In view of the second financing period the large majority of the scientists currently participating in the SPP 1145 agrees that the focus of the SPP 1145 should stay on the development and improvement of first-principles approaches in electronic structure theory. The main emphasis should be on the solution of problems and treatment of effects mainly connected to electron correlation.

3 Participants and Projects

1. *Local ab initio schemes to describe excitons in polymers and solids*
   Martin Albrecht (Siegen)

2. *Wave-function-based correlation method for ground states and excited electron hole and attachment states of periodic systems*
   Uwe Birkenheuer (Dresden)

3. *Wannier-type orbital based Hartree-Fock (-Wigner) electronic structure theory and wavefunction-based correlation treatment for periodic systems*
   Michael Dolg (Köln)

4. *Relativistic Optimized Potential Method for magnetic solids*
   Hubertus Ebert (München)

5. *Density functional theory with implicit functionals: Correlation energy*
   Eberhard Engel (Frankfurt)

6. *Orbital magnetism in molecules and solids*
   Helmut Eschrig, Gotthard Seifert and Manuel Richter (Dresden)

7. *Development of a Relativistic Hilbert-Space Multi-Reference Coupled-Cluster Program*
   Timo Fleig (Düsseldorf)

8. *Accurate wave functions for open-shell atoms including open d- and f-shell elements*
   Stephan Fritzsche (Kassel)

9. *Spin-adapted coupled-cluster theory for the treatment of low-spin open-shell states*
   Jürgen Gauß (Mainz)

10. *Concepts from the optimized potential method and orbital-dependent kernels in time-dependent density-functional theory*
    Andreas Görling (Bonn, since 2004 Erlangen)

11. *A dimension-adaptive sparse grid method for the Schrödinger equation*
    Michael Griebel (Bonn)

12. *Development of a reduced-density-matrix functional theory for solids*
    Eberhard K. U. Groß (Berlin)

13. *Development and application of explicitly-correlated coupled-cluster methods for non-linear optical properties*
    Christof Hättig, Willem Marten Klopper (Karlsruhe)

14. *Development and application of quantum-chemical density-matrix renormalization group methods*
    Bernd A. Heß † (Bonn), continued by Markus Reiher (Jena)

15. *Development and implementation of modern density functional methods for property calculations*
Martin Kaupp (Würzburg)

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)

17. *Development and investigation of orbital functionals in density- and current- density functional theory*
Stefan Kurth (Berlin)

18. *Development of electron structure quantum Monte Carlo methods*
Arne Lüchow (Aachen)

19. *One- to four-component correlated relativistic electronic structure methods based on density matrix renormalization group techniques*
Markus Reiher (Bonn, since 2005 Jena)

20. *Ab initio electron dynamics with the multi-configuration (explicitly) time- dependent Hartree-Fock (MCTDHF) method*
Peter Saalfrank (Potsdam)

21. *First-principle method for the calculation of magnons in real materials*
Leonid M. Sandratskii (Darmstadt)

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

23. *Operator calculus of density matrices and sparse wavelet representations*
Reinhold Schneider (Kiel), Wolfgang Hackbusch and Heinz-Jürgen Flad (Leipzig)

24. *Development of local electron correlation methods for periodic systems*
Martin Schütz (Stuttgart, since 2004 Regensburg)

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)

27. *Coupling of density-functional and configuration-interaction-type methods*
Hermann Stoll and Heinz-Joachim Werner (Stuttgart)

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.

In the group of **M. Albrecht (Siegen)** the project started with a delay in February 2005. Nevertheless important progress has been made in the application of a local incremental scheme to frequency-dependent quantities like the self-energy and hence the Green's function. As a second prerequisite for the progress on the exciton project the problem of infinite lattice summations has been solved analytically and can be incorporated in our approach. Publications for both developments are currently in press (Theor. Chem. Acc., accepted (2005)).

M. Dolg, M. Hanrath (Köln) aim to develop a version of Hartree-Fock-Wigner theory suitable for studies of atoms and molecules as well as polymers and crystals. Initial tests of an existing atom-based parametrization of the correlation kernel on the LiH 3D-crystal yielded satisfactory results. However, in the first molecular applications for a set of about 10 test molecules a relatively poor performance as well as numerical instabilities in the integration routines was observed. As a consequence a new numerically stable HFW-code was written in C++ and the main limitations of the existing ansatz were traced to the symmetric dependence of the correlation kernel on the relative position and momentum. Currently a new more flexible correlation kernel is constructed and schemes to reduce the computational effort are explored, e.g., the point-wise evaluation of the Wigner-intracule and correlation kernel as well as a subsequent two-dimensional integration. In view of a later applicability to solids the so-called incremental scheme based on various types of localized orbitals has been coded thus avoiding the former tedious evaluations "by hand". Last but not least an exponential multi-reference ansatz of the wavefunction has been formulated, implemented in a pilot program and successfully tested on small molecules with strong multi-reference character. A C++ production code is currently written and will be interfaced to the automatized evaluation of the correlation energy by means of an increment expansion. It is hoped that with these tools at hand also periodic systems exhibiting significant multi-reference character, e.g., trans-polyacetylene without bond alternation, can be reliably dealt with.

The formal developments carried out in the group of **H. Ebert (München)** include a consistent formulation of the ROPM-scheme in terms of single particle Green's functions that allow an efficient treatment of core as well as valence electrons on the same footing. Motivated by the work of E. K .U. Gross and S. Kurth H. Ebert and coworkers derived alternative ROPM-equations for the spin-polarised (SDFT) case that improve on numerical efficiency and stability. The program developments led to the first implementation of the SDF-ROPM for spin-polarised atoms. A major step forward in the field of correlated magnetic solids could be achieved by a self-consistent combination of the KKR-method and the DMFT-scheme allowing among other things for the improved description of spectroscopic properties.

The group of **E. Engel (Frankfurt)** work on the analysis and refinement of orbital-dependent correlation energy functionals. As a first step the mathematical analysis of

the 2nd order functional could be completed (Phys. Rev. A, submitted (2005)) and the integral equation for the corresponding 2nd order potential with the appropriate boundary conditions could be solved (J. Chem. Phys., submitted (2005)). By now the formal questions related to orbital-dependent correlation are resolved, so that in the future the emphasis will be on the refinement of this functional and model applications. The second part of the project aims at the relativistic extension of orbital-dependent DFT methods, addressing both Breit and radiative corrections. After establishing the basis for dealing with radiative corrections within DFT (Chem. Phys. 311, 209 (2005)), a DFT representation of the Lamb shift has been derived via a long-wavelength expansion of the QED vertex correction. This work will become the subject of a PhD thesis. The inclusion of Breit corrections has been started, but coding is not yet finished.

For diamagnetic molecules the groups of **H. Eschrig, M. Richter and G. Seifert (Dresden)** have developed and applied a scheme for the calculation of the orbital current induced magnetic field (Chem. Rev. in press (2005)). This result is part of the development of a CDFT for diamagnetic molecules, but it has also found its own application for characterization and visualization of the electronic structure of molecules, especially of aromatic molecules. A systematic derivation of orbital polarization corrections from four-current density functional theory has been found. It can easily be implemented into existing electronic structure codes in order to study the influence of orbital moment contributions in the magnetism of finite and extended systems.

The group of **T. Fleig (Düsseldorf)** completed the interface of the multi-reference coupled-cluster program to the spin-free 4-component Dirac formalism allowing for a number of interesting applications. These include the calculation of complete potential energy curves of molecules of interest in Bose-Einstein condensation experiments, like for instance CsLi and RbYb. For the ground states, these calculations can be carried out to benchmark precision including full iterative triple excitations (CCSDT). The work on the spin-dependent (fully relativistic) implementation is in progress. The MRCC program has been incorporated into the DIRAC program system, the setup and the integral interface have been established. Currently, the relativistic generalization of the evaluation of the CC vector function is being programmed. Furthermore a fully Kramers-restricted and Kramers-adapted relativistic formalism for the general open-shell CC case was derived, which when implemented will allow for exploiting time-reversal symmetry in the many-particle states. The new implementation resulted in collaborations with several theoretical and experimental physicists, i.e., the potential curves and dipole moment function of the CsLi molecule are investigated with P. Schmelcher and M. Pernpointner (Heidelberg). Similar studies are being carried out on the RbYb molecule, a system which plays a role in ultracold molecule experiments at the HHU Dusseldorf by A. Görlitz This project is part of an initiative for a DFG-Forschergruppe under the headship of S. Schiller (Düsseldorf).

B. Fricke (Kassel)[1] and his group have developed a new density functional program which not only uses a full relativistic four-component description, but also includes the effects of the relativistic spin magnetic moments in a self-consistent way. In addition they

[1] B. Fricke acted as the head of the review panel in 2003, but he became now a member of the SPP 1145.

are able to solve the Kohn-Sham equations on the level of a non-collinear description which allows the magnetic moments to point in any direction at every point in space. Strongly improved results were obtained for the binding energies for heavy diatomic molecules and their potential energy curves for tetrachlorides of heavy elements and the magnetic distribution of small magnetic organic systems. Within the SPP 1145 a strong collaboration developed with the group of E. Engel (Frankfurt).

During the last years in the group of **S. Fritzsche (Kassel)** the RATIP program has been developed for studying the level structures and properties of open–shell atoms and ions. For many atomic processes, including the emission and capture of electrons, this program has become today quite a *standard* within the framework of relativistic atomic theory and is well recognized also by other groups in Europe, Asia, and the US. Beside of new developments concerning the stability of relativistic computations or the combination with the density matrix theory, a key request is the maintenance of the code and the support of large–scale computations. During the last five years, in fact, this code has been utilized in more than 50 case studies on various topics of modern electronic structure theory, including Auger (De Fanis et al. 2004, Sienkiewicz et al. 2002, 2003) and photoionization spectra (Huttula et al. 2004), investigations on the coherence transfer (Kitijima et al. 2002), multi–photon ionization (Koval et al. 2003), the analysis of (so–called) 'complete experiments' (O'Keffe et al. 2004), and for several others (Bieron et al. 2004).

The long-term goal of the project of **J. Gauss (Mainz)** and coworkers is the formulation of spin-adapted CC schemes for the treatment of open-shell systems. As an important prerequisite, it was possible in the first project period to formulate and implement general CC methods (for both closed- and open-shell systems) with inclusion of arbitrary excitations in the cluster operator for the treatment of ground-state energies, first- and second-order molecular properties and electronic excited states (via response theory). These developments allow on the one hand calculations of unprecedented accuracy (e.g., 1 kJ/mol in atomization energies, 0.0002 Angstrøm in bond distances, etc.) and on the other hand provide the basic for the future and planned formulation of multi-reference CC methods. For high-spin open-shell molecules, a spin-adapted CC formulation has been already worked out. This approach is currently extended to two-determinantal reference functions. In addition, the size-extensivity problem of partially spin-adapted and rigorously spin-adapted CC schemes is investigated.

The group of **A. Görling (Erlangen)** works on the development of new time-dependent density-functional methods (TDDFT) based on orbital-dependent exchange-correlation kernels. As a first step shortcomings of present TDDFT methods were analysed and it was found that the well-known problem to treat charge-transfer excitations by TDDFT is of a more general nature and occurs generally in weakly coupled system even if no charge-transfer is involved (a publication to be submitted to Chem. Phys. Lett. is currently finalized). It turned out that a solution of this and other problems is only possible with kernels going beyond the commonly applied adiabatic approximation. Therefore the original plan of implementing orbital-dependent but adiabatic kernels was changed and the implementation of the full frequency-dependent exact exchange kernel is now carried out. By casting the underlying formalism in a specific form an implementation strategy

could be developed which make it possible to use existing parts of time-dependent Hartree-Fock methods and thus to somewhat reduce the substantial programming effort. A first implementation step including the computationally most demanding terms of the exact exchange kernel is currently tested.

In the first application period for the project "A dimension-adaptive sparse grid method for the Schr"odinger equation", the group of **M. Griebel (Bonn)** developed sparse grid techniques and product methods for the discretization of Schr"odinger's equation with different choices of multi-level bases (real space, Fourier space) for one-dimensional one-particle states. New and enhanced implementations of the sparse grid approach were realized and a related approach based on separable product expansions was implemented. For the second application period of this SPP, the methods to deal with three-dimensional particle spaces will be improved and applied to atoms, molecules and unit cells of crystals, incorporating antisymmetry, efficient treatment of the Coulomb interaction, dimension-adaptivity and optimal preconditioning of the eigenvalue solver.

The group of **E. Gross (Berlin)** developed a novel method for calculating the fundamental gap as well as photoelectron spectra within Reduced Density Matrix Functional Theory (RDMFT). It was proved that for the exact density matrix functional the Lagrange multiplier used to enforce particle conservation is discontinuous as a function of the (fractional) number of particles. The size of the discontinuity represents the fundamental gap. Electron removal energies, on the other hand, are given by the derivative of the total energy with respect to the corresponding occupation numbers. First numerical results for the chemical hardness of finite systems and for the band gap of periodic solids are very encouraging. Furthermore, RDMFT was extended to open-shell systems by assuming spin-dependent occupation numbers but spin independent natural orbitals. It was shown that, by using spin-resolved chemical potentials, the correlation energy of open-shell atoms is improved significantly (Phys. Rev. Lett., submitted 2005; Phys. Rev. A, Rapid Comm., submitted 2005). In addition it has been demonstrated that the band gap cannot reliably be calculated in DFT, even with the popular EXX approach. The work on periodic solids is based on a marriage of RDMFT with the WANNIER code. This part of the project was performed in close collaboration with M. Albrecht (Siegen). In fact, this collaboration came into existence through the SPP 1145. Since the ultimate goal of the project is to tackle strongly correlated systems, and in particular the high-Tc superconductors, the SPP-funded postdoc, Nektarios Lathiotakis, also worked on an ab-initio approach to superconductors.

During the first financing period **C. Hättig and W. Klopper (Karlsruhe)** have implemented CC-R12 response theory at the level of CC2. The results obtained demonstrate that present implementations of the R12 ansatz lead to problems in the calculation of molecular properties and can become unstable if the (auxiliary) basis sets used in the approximation of three-electron integrals are not carefully chosen. The aim for the next financing period is to modify and generalize the implementation of the R12 ansatz such that it leads to stable and systematically improved results also for molecular properties and excitation energies. It is expected that the outcome of this project will have important implications also for R12 methods presently developed by several groups for ground state

energies.

In the project by **B. Hess † (Bonn)** the analysis and improvement of DMRG convergence has been the major issue. The first systematic study of DMRG parameters (orbital ordering, number of selected states) has been conducted. The main problem in DMRG applications is that no optimum set of reference parameters is available to compare with. This has been solved by the introduction of a genetic algorithm, which provided optimum orbital orderings for the chromium dimer. Results of this work have already been well recognized by the DMRG community and served, for instance, for convergence acceleration in a recent study by Chan. The extensive tests, which have been carried out in this project, shed light on the strong and weak points of the DMRG algorithm. Having the weak points clearly identified, directions for future research are now much clearer than in 2003 when the project began. After the death of B. Hess in summer 2004 the project was supervised by M. Reiher (Bonn, now Jena).

The group of **M. Kaupp (Erlangen)** completed the implementation of an OEP-Ansatz (LHF and KLI approximations) into the ReSpect program successfully, both for the closed- and open-shell cases. This has allowed the test of "localized hybrid potentials" for the calculation of various NMR and EPR parameters, with extremely promising results. In particular, the best agreement with experiment has been achieved with relatively high exact-exchange admixtures of about 0.5-0.6. Remarkably, this holds for both chemical shifts of main group compounds and g-tensors of transition metal complexes. Currently ongoing further developments, which are expected to provide a new generation of exchange-correlation potentials for property calculations are a) work towards the first self-consistent implementation of "local hybrid functionals" with position-dependent exact-exchange admixtures and b) the first self-consistent implementation of Becke's recent real-space model of nondynamical correlation. New collaborations have developed within the SPP with a) A. Görling and W. Hieringer (Erlangen) on OEP models and localized hybrid potentials, and have been started recently with S. Kurth (Berlin) on current density functional theory. Due to the workshop on OEP in Berlin, contacts with S. Kümmel (Dresden) on local hybrid functionals were established.

The group of **W. Klopper (Karlsruhe)** has shown that it is possible to compute analytically the effective density matrix that is needed to compute first-order one-electron molecular properties from its trace with the corresponding one-electron property matrix (J. Chem. Phys. 122, 214306 (2005)). The construction of this effective density matrix is a first step towards the development of the analytic calculation of nuclear gradients of explicitly correlated methods, which is their ultimate goal. They have not only developed the calculation of this effective density matrix , but also developed further the explicitly correlated methods themselves. They have introduced the resolution-of-identity approximation of Manby (sometimes called density-fitting approach) as well as the Slater-type geminal of Ten-no (J. Phys. B: At. Mol. Opt. Phys. (in press)). A future highlight would be the analytic calculation of nuclear gradients not only of the original but also, if possible, of the improved explicitly correlated methods.

The research group of **S. Kurth (Berlin)** started with a project on the theory and implementation of the optimized effective potential (OEP) method in current-density func-

tional theory (CDFT) developed originally by N. Helbig and E.K.U. Gross for the collinear case. They generalized the OEP equations to the non-collinear case and rewrote them in a more compact and transparent form. A numerical scheme for the approximate solution of the OEP equations was devised and implemented for open-shell atoms at the exchange-only level in order to investigate if the spurious lifting of degeneracies for different ground states which is found in spin-DFT is alleviated in CDFT. Unfortunately, this is not the case, the splittings actually being increased in CDFT. It was surprising, however, that in DFT, i.e., when *only* the density is used as fundamental variable, the different ground-state configurations indeed lead to degenerate ground-state energies.

A. Lüchow (Aachen) and coworkers performed quantum Monte Carlo calculations on ground and excited states of the carbon atom, ethene, and formaldehyde, and on the ground state of transition metal carbonyls. They analyzed the different energies for different nodal regions, could identify spurious nodal regions and analyzed their importance for the quantum Monte Carlo process. The first quantum Monte Carlo calculations for Rydberg states have been obtained in collaboration with A. Görling and F. Della Sala who provided orbitals from their localized HF method. Finally, the quantum Monte Carlo code has been reworked and improved considerably.

The project of **M. Reiher (Jena)** on DMRG is dealing with another feature of the DMRG algorithm, which is the form and construction of the many-electron operator that is determined the number of states available per site. In other words, it deals with relativistic Hamiltonians which require a variable number of states per site. Because of the explicit matrix representation of all creation and annihilation operators in DMRG, the number of states available requires a flexible implementation, which was not available and which is now under constant development. Since the total number of sites is a crucial factor for DMRG convergence, it was necessary to restrict the number of orbitals to be taken into account to a large extent. For this purpose, the infinite-order Douglas–Kroll–Hess (DKH) scheme has been developed, which does not make any reference to a small-component of the molecular spinor. It thus avoids large basis sets which would in turn lead to a large number of one-particle states. This infinite-order DKH scheme is an innovative and new development essential for the relativistic DMRG program but it is also a valuable general spin-off of the project. The MOLPRO implementation of the new DKH algorithm has served as a basis for the first relativistic DMRG study on CsH. The potential curve of CsH represents an interesting test case of sufficient complexity to point to necessary improvements of the DMRG algorithm. Consequently, new warm-up procedures are now being introduced in order to efficiently generate the crucial environment states for the very first DMRG iteration steps. From the work within the SPP 1145 also a paper on higher-order Douglas–Kroll–Hess electric field gradient calculations emerged as a collaboration of F. Neese and the SPP 1145 projects by M. Reiher, by B. A. Hess, and by T. Fleig (J. Chem. Phys. 122, 204107 (2005)).

P. Saalfrank, T. Klamroth (Potsdam) and coworkers implemented the explicitly time-dependent Multi-Configuration Self-Consistent Field method, and used it to simulate correlated many electron dynamics in model systems. Also, they implemented interface routines in order to connect our quantum dynamics programs with the GAMESS quantum

chemistry package, which was used already for three-dimensional time-dependent CI calculations. In future they plan to turn to real, three-dimensional systems, also for MCTDHF. The group is also cooperating with E.K.U. Gross, who has much experience with electron dynamics using the time-dependent DFT approach and applications to unbound problems, such as laser ionization of atoms. On a longer timescale a collaboration with other groups of the SPP, in particular on the interfacing of MCTDHF with efficient quantum chemistry programs is intended. An interesting exchange of ideas originated at the workshop in Kiel, where they learned about the generation of highly optimized FORTRAN/C code using Maple. The discussions at the SPP 1145 workshop were very useful.

A. Schindlmayr, G. Bihlmayer, S. Blügel (Jülich) and coworkers completed an all-electron implementation of the GW approximation within the full-potential linearized augmented plane-wave (FLAPW) method. It allows ab initio calculations of quasiparticle excitations for materials that are not accessible by earlier plane-wave pseudopotential codes, such as magnetic transition metals. Special emphasis was placed on a careful analysis of the influence of the FLAPW basis set, and systematic improvements for higher-lying conduction bands were proposed. In advance of the planned extension to spin-wave excitations, the single-particle Stoner contribution to the transverse spin susceptibility and interaction matrix elements between localised d-electrons have already been obtained from first principles.

In the groups of **W. Hackbusch, H.-J. Flad (Leipzig) and R. Schneider (Kiel)** the operator calculus of density matrices and sparse wavelet representations is studied. A multiresolution approach to linear scaling methods for Hartree-Fock and Kohn-Sham equations was suggested based on wavelet representations of density matrices and Fock operators. Within the first period of the priority program sparse wavelet representations of one-electron density matrices using best N-term approximation theory has been studied. (Mathematical modelling and numerical analysis (ESAIM), submitted (2005)). This work has been recently extended to Jastrow-type correlation functions (Mathematical modelling and numerical analysis (ESAIM), to be submitted (2005)). Furthermore they have investigated hierarchical Kronecker tensor product approximations to electron densities, where individual components of the tensor products are efficiently represented in wavelet bases. The tensor product structure greatly simplifies the adaptive computation of Hartree potentials and exchange operators (Z. Num. Math., submitted (2005)). This part of the project has also some relevance for local correlation methods which will be pursued in collaboration with M. Schütz (Regensburg). Further applications of separable approximations (IMA J. Numer. Anal., accepted for publication (2005)) have been studied in collaboration with J. Gauss (Mainz) and M. Albrecht (Siegen).

In the course of the SPP project a close collaboration between the group of **M. Schütz (Regensburg)** and the authors of the widely used CRYSTAL program package in Torino in particular, C. Pisani, was established. Recently, a pilot implementation of a periodic local MP2 method has been reported (J. Chem. Phys. 122, 094113, 2005). The point group symmetry of the crystal was properly exploited in this program (a prerequisite for an efficient treatment of crystals, which usually have rich symmetry). Nevertheless, the computational cost for treating true 3-D systems turned out to be rather high and

only small and simple systems could be treated. In the meantime, however, substantial progress has been made: Density Fitting was introduced, which turned out to be essential for an efficient treatment of electron correlation in crystals by use of local correlation methods. Translational symmetry is utilized extensively: for example, the calculation of fitting coefficients and the assembly of the required electron repulsion integrals proceeds in Fourier space. Convergence problems in the context of the Fourier transform could be avoided by virtue of Poisson fitting functions. Their present periodic local MP2 program is about three orders of magnitude faster than the original pilot program reported before (10 minutes instead of 3 weeks for a calculation on diamond). As a sideline of the project, Usvyat and Schütz investigated possibilities to generate and exploit ultralocalized (non-orthogonal) Wannier functions (Theor. Chem. Accounts, in press). The use of such ultralocalized functions in the context of their MP2 program is currently explored. A further milestone of the project for the second application period is the implementation of a local CCSD program.

The group of **G. Soff † and G. Plunien (Dresden)** focusses on ab-initio QED calculations of spectra and transition probabilities in atomic systems. They have solved the problem due to the occurrence of spurious states in finite-basis-set representations of the Dirac spectrum (Phys. Rev. Lett. 93, 130405 (2004)) Utilizing a specific basis - termed as *dual kinetically balanced* - for the radial part of the Dirac wave functions, one can prove explicitly the absence of spurious states. As a crucial point, the ansatz employed for the Dirac spinors for positive and negative energy states respect the symmetry of charge conjugation. The progress achieved is evident: The acceleration of the convergence due to the absence of spurious states from the very beginning allows the evaluation of higher-order QED corrections in few-electron systems (bound-state QED methods) with increasing efficiency. The generalization of this finite-basis-set approach to non-Coulomb potentials allows for making contact as well with self-consistent schemes employed in many-electron systems. The *dual kinetic balance approach* will be employed in all future QED calculations for atomic many-electron systems. The *line profile approach* (LPA) was applied for the evaluation of energy levels in He-like and Li-like HCI (Nucl. Instr. Meth. B 205, 25 (2003); Phys. Rev. A 67, 012503 (2003); Phys. Rev. A 69, 062505 (2004)). The result obtained can be presently considered as the most accurate ones. The most general formulation of the LPA for many-electron systems, which is also applicable for the description of quasi-degenerate levels has been developed Phys. Rev. A 69, 062505 (2004)). A most recent compilation of complete results for QED corrections in He-like ions as well as for the screened self-energy correction to the transition energy in Li-like ions has been provided on the basis of the *two-time Green function method* (Phys. Rev. A (2005), in press; Phys. Lett. A 316, 395 (2003). Electron-correlation effects in atoms and ions can be tested in dynamic processes, where the interelectronic interaction plays a crucial role. E.g. double-photoionization/-recombination with a single real photon can take place only due to interelectron interactions mediated by the exchange of virtual photons. Accordingly, they have investigated double K-shell ionization of heliumlike ions (Phys. Lett. A 316, 395 (2003), Phys. Rev. A 69, 032703 (2004), Phys. Lett. A 328, (2004) 350) so far mainly within the nonrelativistic domain. To extend such ab-initio QED calculations also to many-

electron ions and atoms is intended. Highlighting the tasks achieved and the future goals in brief: The tools and methods at hand provide a firm basis of performing ab-initio QED calculations for atomic many-electron systems in accordance with the tasks and scope of the DFG priority program 1145. Moreover, they are aiming for tests of fundamental interactions in atomic systems (parity nonconservation effects, fundamental symmetries (PCT theorem), time-dependence of fundamental parameters (Phys. Rev. Lett. 94 (2005)). A new collaboration with S. Fritzsche (University of Kassel) will strengthen the existing close collaborations with L. Labzowsky and V. Shabaev from the St. Petersburg State University and A. Mikhailov from the St. Petersburg Nuclear Physics Institute.

H. Stoll, H.-J. Werner (Stuttgart) and coworkers aim at coupling density-functional (DFT) and wavefunction-based ab-initio methods, by separating the interelectronic interaction into a short-range part which is treated by DFT, and a long-range part which is treated by ab-initio methods with explicit account of electron correlation. The highest level which has been achieved within the present application period (DFT with a newly optimized gradient-corrected Perdew-Burke-Ernzerhof-(PBE-)like functional, coupled to an ab-initio coupled-cluster treatment with single and double excitations and perturbative account of triples (CCSD(T)) shall be extended from closed-shell to high-spin open-shell reference wavefunctions. In addition, the computational efficiency of the long-range ab-initio treatment shall be improved by invoking local-correlation methods and applying multipole and Fourier-transform techniques. New collaborations with J. Angyan (Nancy) and H. J. Aa. Jensen (Odense) were stimulated by the project.

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. Other publications on topics relevant to the SPP 1145, but not being a direct outcome of the SPP 1145 are not listed.

1. *Towards a frequency independent incremental ab initio scheme for the self energy*, M. Albrecht, Theor. Chem. Acc., accepted (2005).
2. *Implicit intinite lattice summations for real space ab initio correlation methods*, M. Albrecht, Theor. Chem. Acc., accepted (2005).
3. *Evaluation of the low-lying energy levels of the two- and three-electron configurations for multicharged ions*, O. Yu. Andreev, L. N. Labzowsky, G. Plunien and G. Soff, Phys. Rev. A 67, 012503 (2003).
4. *Calculation of quasi-degenerate energy levels of two-electron multi-charged ions*, O. Yu. Andreev, L. N. Labzowsky, G. Plunien and G. Soff, Phys. Rev. A 69, 062505 (2004).
5. *Testing the time dependence of fundamental constants in the spectra of multicharged ions*, O. Yu. Andreev, L. N. Labzowsky, G. Plunien, G. Soff, Phys. Rev. Lett. 94 (2005).
6. *Improved density functional calculations including magnetic effects for $RfCl_4$ and its homologues*, J. Anton, M. Hirata, B. Fricke, V. Pershina, Chem. Phys. Lett. 380, 95 (2003).
7. *Non-collinear and collinear relativistic density-functional program for electric and magnetic properties of molecules*, J. Anton, B. Fricke, E. Engel, Phys. Rev. A 69, 012505 (2004).
8. *An ab-initio study of the magnetic ground states of organic molecules of di- resp. tetramethyl types as examples with a non-collinear density functional method*, J. Anton, T. Ishii, B. Fricke, Chem. Phys. Lett. 388, 248 (2004).
9. *Non-collinear and collinear four-component relativistic molecular density functional calculations*, J. Anton, B. Fricke, P. Schwerdtfeger, Chem. Phys. 311, 97 (2005).
10. *Local Hybrid Exchange-Correlation Potentials for Kohn-Sham DFT Calculations of NMR and EPR Parameters*, A. V. Arbuznikov, M. Kaupp, Int. J. Quantum Chem. 102, 261 (2005).
11. *Unrestricted open-shell Kohn-Sham scheme with local hybrid exchange-correlation potentials. Improved calculation of electronic g-tensors for transition-metal complexes*, A. V. Arbuznikov, M. Kaupp, Chem. Phys. Lett. 391, 16 (2004).
12. *Construction of local hybrid exchange-correlation potentials. Evaluation for nuclear shielding constants*, A. V. Arbuznikov, M. Kaupp, Chem. Phys. Lett. 386, 8 (2004).
13. *The self-consistent implementation of exchange-correlation functionals depending on the local kinetic energy density*, A. V. Arbuznikov, M. Kaupp, Chem. Phys. Lett. 381, 495 (2003).

14. *QED calculation of the $n = 1$ and $n = 2$ energy levels in He-like ions*, A. N. Artemyev, V. M. Shabaev, V. A. Yerokhin, G. Plunien, G. Soff, Phys. Rev. A 71, 062104 (2005).
15. *Fast computation of adaptive wavelet expansions*, A. Barinka, W. Dahmen, R. Schneider, Z. Num. Math, submitted (2005).
16. *Equation-of-Motion Coupled-Cluster Methods for Ionized States with an Approximate Treatment of Triple Excitations*, Y. Bomble, J.C. Saeh, J.F. Stanton, P.G. Szalay, M. Kallay, J. Gauss, J. Chem. Phys. 122, 154107-1 (2005).
17. *Coupled-Cluster Methods including Non-Iterative Corrections for Quadruple Excitations*, Y. Bomble, J.F. Stanton, M. Kallay, J. Gauss, J. Chem. Phys., accepted (2005).
18. *Approximation of $1/x$ by exponential sums in $[1, \infty)$*, D. Braess and W. Hackbusch, IMA J. Numer. Anal. accepted (2005).
19. *Sparse grids*, H.-J. Bungartz, M. Griebel. *Acta Numerica*, 13:1–123 (2004).
20. *Induced magnetic fields in aromatic annulenes*, C. Corminboeuf, Th. Heine, G. Seifert, P. Schleyer, J. Weber, Phys. Chem. Chem. Phys. 6, 273 (2004).
21. *Monte Carlo for the first dissociation energies of transition metal carbonyls*, C. Diedrich, A. Lüchow, S. Grimme, J. Chem. Phys. 122, 21101 (2005).
22. *Exchange-correlation and QED effects from a density functional based level shift approach*, E. Engel, U. Lechner, Chem. Phys. 311, 209 (2005).
23. *Solubility of the OPM integral equation for finite systems*, E. Engel, H. Jiang, A. Facco Bonetti, Phys. Rev. A., submitted (2005).
24. *Second order correlation potential of atoms in cavity*, E. Engel, H. Jiang, J. Chem. Phys., submitted (2005).
25. *Best N-term approximation in electronic structure calculations.I. One-electron reduced density matrix*, H.-J. Flad, W. Hackbusch, R. Schneider, Mathematical modelling and numerical analysis (ESAIM), submitted (2005).
26. *Coupled-cluster theory with simplified linear r_{12} corrections: The CCSD(R12) model*, H. Fliegl, C. Hättig, W. Klopper, J. Chem. Phys. 122, 084107 (2005).
27. *Superconducting properties of MgB2 from first principles*, A. Floris, G. Profeta, N.N. Lathiotakis, M. Lueders, M.A.L. Marques, C. Franchini, E.K.U. Gross, A. Continenza, S. Massidda, Phys. Rev. Lett. 94, 037004 (2005).
28. *Molecular results for Hartree-Fock-Wigner theory*, R. Fondermann, M. Hanrath, M. Dolg, D. O'Neill, Chem. Phys. Lett., submitted (2005).
29. *Coupling of short-range GGA with long-range coupled-cluster methods*, E. Goll, H.-J. Werner, H. Stoll, submitted (2005).
30. *An Exponential Multi-Reference Wavefunction Ansatz*, M. Hanrath, J. Chem. Phys., in press (2005).
31. *Equilibrium Geometries based on Coupled-Cluster Calculations involving Quadruple Excitations*, M. Heckert, M. Kallay, J. Gauss, Mol. Phys., accepted (2005).
32. *Spin-Adapted Coupled-Cluster Theory for High-Spin Open-Shell States*, M. Heckert, O. Heun, J. Gauss, P.G. Szalay, J. Chem. Phys., submitted for publication (2005).

33. *The magnetic shielding function of molecules and pi electron delocalization*, Th. Heine, C. Corminboeuf, G. Seifert, Chem. Rev., in press (2005).
34. *The fundamental gap in reduced density matrix functional theory*, N. Helbig, N.N. Lathiotakis, M. Albrecht, E.K.U. Gross, Phys. Rev. Lett., submitted (2005).
35. *Analytic Second Derivatives for General Coupled-Cluster and Configuration-Interaction Models*, M. Kallay and J. Gauss, J. Chem. Phys 120, 6841 (2004).
36. *Calculation of Excited-State Properties using General Coupled-Cluster and Configuration-Interaction Models*, M. Kallay and J. Gauss, J. Chem. Phys. 121, 9257 (2004).
37. *Analytic calculation of first-order molecular properties at the explicitly correlated second-order Møller-Plesset level: Basis-set limits for the molecular quadrupole moments of BH and HF*, E. Kordel, C. Villani, and W. Klopper, J. Chem. Phys. 122, 214306 (2005).
38. *Time-dependent configuration interaction calculation of laser-pulse driven many-electron dynamics: Controlled dipole switching in lithium cyanide*, P. Krause, T. Klamroth, and P. Saalfrank, J. Chem. Phys., in press (2005).
39. *Density functional theory for superconductors*, N.N. Lathiotakis, M.A.L. Marques, M. Lueders, L. Fast, and E.K.U. Gross, Int. J. Quant. Chem. 99, 790 (2004).
40. *Open shells in reduced-density-matrix-functional theory*, N.N. Lathiotakis, N. Helbig, E.K.U. Gross, Phys. Rev. A, Rapid Comm., submitted (2005).
41. *Ab-initio theory of superconductivity - I: Density functional formalism and approximate functionals*, M. Lueders, M.A.L. Marques, N.N. Lathiotakis, A. Floris, G. Profeta, L. Fast, A. Continenza, S. Massidda, E.K.U. Gross, Phys. Rev. B, accepted (2005).
42. *Exact-exchange density-functional calculations for noble-gas solids*, R.J. Magyar, A. Fleszar, E.K.U. Gross, Phys. Rev. B 69, 045111 (2004).
43. *Ab-initio theory of superconductivity - II: Applications to elemental metals*, M.A.L. Marques, M. Lueders, N.N. Lathiotakis, G. Profeta, A. Floris, L. Fast, A. Continenza, E.K.U. Gross, S. Massidda, Phys. Rev. B, accepted (2005).
44. *The induced magnetic field in cyclic molecules*, G. Merino, Th. Heine, G. Seifert, Chemistry - A European Journal 10, 4367 (2004).
45. *Nondipole effects in double K-shell ionization of heliumlike ions*, A. I. Mikhailov, I. A. Mikhailov, A. N. Moskalev, A. V. Nefiodov, G. Plunien and G. Soff, Phys. Lett. A 316, 395 (2003)
46. *Nonrelativistic double photoeffect on K-shell electrons*, A. I. Mikhailov, I. A. Mikhailov, A. N. Moskalev, A. V. Nefiodov, G. Plunien and G. Soff, Phys. Rev. A 69, 032703 (2004)
47. *Correlated double electron capture with a single photon*, A. I. Mikhailov, I. A. Mikhailov, A. V. Nefiodov, G. Plunien, G. Soff, Phys. Lett. A 328, (2004) 350.
48. *Multiple scattering formalism for correlated systems: A KKR+DMFT approach*, J. Minár, L. Chioncel, A. Perlov, H. Ebert, M. I. Katsnelson, A. I. Lichtenstein, Phys. Rev. B, accepted (2005).

49. *Convergence Behavior of the Density Matrix Renormalization Group Algorithm for Optimized Orbital Orderings*, G. Moritz, B. A. Hess, M. Reiher, J. Chem. Phys. 122, 024107 (2005).
50. *Relativistic DMRG calculations on the curve crossing of cesium hydride*, G. Moritz, A. Wolf, M. Reiher, J. Chem. Phys., submitted (2005).
51. *Calculation of Electric Field Gradients based on Higher-Order Generalized Douglas–Kroll Transformations*, F. Neese, A. Wolf, T. Fleig, M. Reiher, B. A. Hess, J. Chem. Phys. 122, 204107 (2005).
52. *The Multi-Configuration Time-Dependent Hartree-Fock method for quantum chemical calculations*, M. Nest, T. Klamroth, and P. Saalfrank, J. Chem. Phys. 122, 124102 (2005).
53. *Correlated many electron dynamics: Application to inelastic electron scattering at a metal film*, M. Nest and T. Klamroth, Phys. Rev. A, in press (2005).
54. *Planar Tetracoordinate Carbons in Cyclic Hydrocarbons*, N. Perez, Th. Heine, R. Barthel, G. Seifert, A. Vela, M.A. Mendez-Rojas, G. Merino, Organic Letters 7, 1509 (2005).
55. *Local-MP2 electron correlation method for non conducting crystals*, C. Pisani, M. Busso, G. Capecchi, S. Casassa, R. Dovesi, L. Maschio, C. Zicovich-Wilson, M. Schütz, J. Chem. Phys. 122, 094113 (2005).
56. *Exact decoupling of the Dirac Hamiltonian. I. General Theory*, M. Reiher, A. Wolf, J. Chem. Phys. 121, 2037 (2004).
57. *Exact Decoupling of the Dirac Hamiltonian. II. The generalized Douglas–Kroll–Hess transformation up to arbitrary order*, M. Reiher, A. Wolf, J. Chem. Phys. 121, 10945 (2004).
58. *Laser-driven electron dynamics at interfaces*, P. Saalfrank, T. Klamroth, C. Huber, and P. Krause, Isr. J. Chem. 45, 205 (2005).
59. *Magnetic properties of Co impurities in bulk Au: DFT calculations*, M. Sargolzaei, I. Opahle, M. Richter, K. Koepernik, U. Nitzsche, H. Eschrig, J. Magn. Magn. Mat. 290-291, 364 (2005).
60. *Dual kinetic balance approach to basis-set expansions for the Dirac equation*, V. M. Shabaev, I. I. Tupitsyn, V. A. Yerokhin, G. Plunien, and G. Soff, Phys. Rev. Lett. 93, 130405 (2004).
61. *Northogonal ultralocalized functions and fitted Wannier functions for local correlation methods for solids*, D. Usvyat, M. Schütz, Theor. Chem. Acc., in press (2005).
62. *Explicitly-correlated calculation of the second-order Møller-Plesset correlation energies of Zn2+ and Zn*, C. Villani and W. Klopper, J. Phys. B: At. Mol. Opt. Phys, in press (2005).
63. *Screened self-energy corrections to the $2p_{3/2} - 2s$ transition energy in Li-like ions*, V. A. Yerokhin, A. N. Artemyev, V. M. Shabaev, G. Plunien, G. Soff, Optics and Spectroscopy 99, 12 (2005).

6 Symposia and Workshops

6.1 Symposia

The initial symposium and review panel meeting 2003 as well as the second symposium 2004 were both held in Bonn. The third symposium and second panel meeting will also take place in Bonn in 2005.

It is planned that the 2006 symposium will be organized by Hans-Joachim Werner (Stuttgart) and Jürgen Gauss (Mainz) in Bad Herrenalb in June 2006.

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 (status June 28, 2005)

34 project proposals will be presented on posters, 24 being renewal proposals and 10 new proposals. Similar to the symposium in 2003 the new proposals will be described in oral presentations of 10 minutes each (including discussion). A selection of the renewal proposals will be 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 have been invited for lectures.

6.1.4 Programs and lists of participants of the symposia 2003 - 2005

First Meeting of the DFG Priority Program 1145
June 1-3, 2003, CJD Bonn
Program (May 26, 2003)

Please note that the actual program will depend on the demands of the members of the review panel. The following program outline is thus subject to possible changes.

Sunday June 1, 2003

until 5:00 p.m.	Arrival of project applicants, reviewers, guests
from 5:00 p.m.	Project applicants should put their posters on display (cf. the list of talks for the number of the poster)
5:00-5:30 p.m.	First meeting of the review panel board (together with Dr. Kuchta, DFG)
6:00 p.m.	Dinner

Monday June 2, 2003 *

	Breakfast
8:45 a.m.	Welcome (Dr. Kuchta, DFG; Prof. Dr. Dolg, Cologne)
9:00 a.m. - 10:30 a.m.	Short oral project presentations I
10:30 a.m. - 11:00 a.m.	Coffee break
11:00 a.m. - 12:30 a.m.	Short oral project presentations II
12:30 a.m. - 2:00 p.m.	Lunch
2:00 p.m. - 3:30 p.m.	Short oral project presentations III
3:30 p.m. - 4:00 p.m.	Coffee break
4:00 p.m. - 5:30 p.m.	Short oral project presentations IV
5:30 p.m.	Second meeting of the review panel board
6:00 p.m.	Dinner
	Discussion of the project applicants with the members of the review panel board at the posters (if required by the review panel)

* Please refer to the detailed timetable on the next page !

Tuesday June 3, 2003

	Breakfast
from 9:00 a.m.	Third meeting of the review panel board
9:00 a.m. - 10:00 a.m.	Discussion of the project applicants about future directions of the DFG priority program 1145
from 10:00 a.m.	Discussion of the project applicants with the members of the review panel board at the posters (if required by the review panel)
12:30 a.m.	Lunch
	Departure

Table 1: Timetable of presentations (5 minutes presentation plus 5 minutes discussion)

morning (a.m.)								
8:45	Welcome							
9:00	V1 Albrecht	10:00	V7 Fleig	11:00	V10 Görling	12:00	V16 Kaupp	
9:10	V2 Birkenheuer	10:10	V8 Fritzsche	11:10	V11 Griebel	12:10	V17 Ebert	
9:20	V3 Dolg	10:20	V9 Gauß	11:20	V12 Grimme	12:20		
9:30	V4 Engel	10:30	Coffee Break	11:30	V13 Groß	12:30	Lunch	
9:40	V5 Engels			11:40	V14 Hättig			
9:50	V6 Eschrig			11:50	V15 Heß			
afternoon (p.m.)								
2:00	V18 Soff	3:00	V24 Redmer	4:00	V27 Sandratskii	5:00	V33 Springborg	
2:10	V19 Klopper	3:10	V25 Reiher	4:10	V28 Schindlmayr	5:10	V34 Stoll	
2:20	V20 Klimer	3:20	V26 Saalfrank	4:20	V29 Schirmer	5:20		
2:30	V21 Kolb	3:30	Coffee Break	4:30	V30 Schneider	5:30	Dinner,	
2:40	V22 Kurth			4:40	V31 Schütz		Meeting of the	
2:50	V23 Lüchow			4:50	V32 Seidl		Review Panel	
evening								
Poster Session, Discussion between Applicants and Members of the Review Panel (depending on the actual demands of the latter)								

Talks are in alphabetical order of names of (main/first) applicants,
except V17 (due to late arrival on Monday) and V18 (due to early departure on Monday).
The name of the actual project presenter may differ from the name listed.
Please note: the number of the talk denotes also the number of the poster.

First Symposium and Review Panel Meeting of the DFG priority program 1145 June 1 - 3, 2003, CJD Bonn

Participants:

1. Prof. Dr. Martin Albrecht, Siegen
2. Prof. Dr. Stefan Blügel, Jülich
3. Dr. Uwe Birkenheuer, Dresden
4. Prof. Dr. Michael Dolg, Köln
5. Prof. Dr. Hubert Ebert, München
6. Prof. Dr. Bernd Engels, Würzburg
7. Priv.-Doz. Eberhard Engel, Frankfurt
8. Prof. Dr. Helmut Eschrig, Dresden
9. Dr. Manuel Richter, Dresden
10. Prof. Dr. Gotthard Seifert, Dresden
11. Dr. Timo Fleig, Düsseldorf
12. Priv.-Doz. Dr. Stephan Fritzsche, Kassel
13. Prof. Dr. Jürgen Gauß, Mainz
14. Prof. Dr. Andreas Görling, Bonn
15. Prof. Dr. Michael Griebel, Bonn
16. Prof. Dr. Eberhard Groß, Berlin
17. Prof. Dr. Stefan Grimme, Münster
18. Dr. Christof Hättig, Karlsruhe
19. Prof. Dr. Willem Klopper, Karlsruhe
20. Prof. Dr. Bernd Artur Hess, Erlangen
21. Prof. Dr. Martin Kaupp, Würzburg
22. Dr. Thorsten Klüner, Berlin
23. Prof. Dr. Dietmar Kolb, Kassel
24. Dr. Stefan Kurth, Berlin
25. Priv.-Doz. Dr. Arne Lüchow, Aachen
26. Prof. Dr. Ronald Redmer, Rostock
27. Priv.-Doz. Dr. Markus Reiher, Erlangen
28. Prof. Dr. Peter Saalfrank, Potsdam
29. Dr. Tilmann Klamroth, Potsdam
30. Priv.-Doz. Dr. Leonid Sandratskii, Halle
31. Prof. Dr. Jochen Schirmer, Heidelberg
32. Dr. Arno Schindlmayr, Jülich
33. Dr. G. Bihlmayer, Jülich
34. Prof. Dr. R. Schneider, Chemnitz
35. Dr. Heinz-Jürgen Flad, Leipzig
36. Prof. Dr. Wolfgang Hackbusch, Leipzig

37. Priv.-Doz. Dr. Martin Schütz, Stuttgart
38. Priv.-Doz. Dr. Michael Seidl, Regensburg
39. Prof. Dr. Gerhard Soff, Dresden
40. Prof. Dr.-Ing. Michael Springborg, Saarbrücken
41. Prof. Dr. Hermann Stoll, Stuttgart
42. Prof. Dr. Hans-Joachim Werner, Stuttgart

Review Panel:

1. Prof. Dr. Knut Faegri, Oslo
2. Prof. Dr. Burkhard Fricke, Kassel
3. Prof. Dr. Peter M. W. Gill, Nottingham
4. Prof. Dr. Poul Joergensen, Arhus
5. Prof. Dr. Werner Kutzelnigg, Bochum
6. Prof. Dr. A. I. Lichtenstein, Nijmegen
7. Prof. Dr. Dominik Marx, Bochum
8. Prof. Dr. Risto Nieminen, Helsinki
9. Prof. Dr. Walter Thiel, Mülheim

Guests:

1. Dr. Bischler, Volkswagenstiftung
2. Dr. Fuchs, Berlin
3. Prof. Dr. Georg Jansen, Essen
4. Dr. Kratzer, Berlin
5. Dr. Beate Paulus, Dresden

MODERN AND UNIVERSAL FIRST-PRINCIPLES-METHODS FOR MANY-ELECTRON SYSTEMS IN CHEMISTRY AND PHYSICS

CJD Bonn, Graurheindorfer Str. 149, 53117 Bonn, Tel. 0228/98960, http://www.cjd-bonn.de
May 24, 2004 – May 25, 2004

Agenda

Monday, May 24, 2004

12:00 Lunch

13.30–14.00 **Andreas Görling** (Bonn) :
Orbital- and state-dependent functionals in DFT I
14.00–14.10 Discussion

14.10–14.40 **Eberhard Engel** (Frankfurt) :
Orbital- and state-dependent functionals in DFT II
14.40–14.50 Discussion

14.50 COFFEE BREAK

15.30–16.00 **Hubert Ebert** (München) :
Application of the Optimized Potential Method to magnetic solids — formalism and implementation
16.00–16.10 Discussion

16.10–16.40 **Martin Albrecht** (Siegen) :
Ab initio methods for electronic correlation in solids: an overview
16.40–16.50 Discussion

17.30 DINNER

19.00 **POSTER SESSION**

Tuesday, May 25, 2004

09.00–09.30 **Reinhard Noack** (Marburg) :
The Density Matrix Renormalization Group: Overview and Prospects
09.30–09.40 Discussion

09.40–10.10 **Peter M. W. Gill** (Nottingham) :
Hartree–Fock–Wigner models for electron correlation
10.10–10.20 Discussion

10.20 COFFEE BREAK

11.00–11.30 **Wim Klopper** (Karlsruhe) :
Coupled-cluster theory with linear r_{12} terms
11.30–11.40 Discussion

11.40–12.10 **Poul Jørgensen** (Aarhus) :
Response function theory for coupled cluster wave functions
12.10–12.20 Discussion

12.30 LUNCH

14.30–15.00 **Wolfgang Hackbusch** (Leipzig) :
Separable Approximations
15.00–15.10 Discussion

15.10–15.40 **Stephan Fritzsche** (Kassel) :
How well do we understand the properties and level structures of atoms?
15.40–15.50 Discussion

15.50 COFFEE BREAK

16.30–17.00 **Arne Lüchow** (Aachen) :
Quantum Monte-Carlo methods in chemistry
17.00–17.10 Discussion

17.10–17.40 **Peter Saalfrank** (Potsdam) :
Theoretical treatment of ultrafast processes at interfaces
17.40–17.50 Discussion

18.00 DINNER

Second Meeting of the DFG Priority Program 1145

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

May 24 - 25, 2004

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

Participants

1. Albrecht, Martin (Siegen)
2. Anton, Josef (Kassel)
3. Arbuznikov, Alexei V. (Würzburg)
4. Bihlmayer, Gustav (Jülich)
5. Birkenheuer, Uwe (Dresden)
6. Bringer, Andreas (-)
7. Dolg, Michael (Köln)
8. Elhajal, Maged (Halle)
9. Engel, Eberhard (Frankfurt)
10. Flad, Heinz-Jürgen (Leipzig)
11. Fleig, Timo (Düsseldorf)
12. Fliegl, Heike (Karlsruhe)
13. Fondermann, Rebecca (Köln)
14. Fricke, Burkhard (Kassel)
15. Friedrich, Christoph (Jülich)
16. Fritzsche, Stephan (Kassel)
17. Fuchs, Martin (Berlin)
18. Gauss, Jürgen (Mainz)
19. Gill, Peter (Nottingham, UK)
20. Goll, Erich (Stuttgart)
21. Görling, Andreas (Erlangen)
22. Hackbusch, Wolfgang (Leipzig)
23. Hamaekers, Jan (Bonn)
24. Hanrath, Michael (Köln)
25. Hättig, Christof (Karlsruhe)
26. Helbig, Nicole (Berlin)
27. Heckert, Miriam (Mainz)
28. Heß, Bernd (Bonn)
29. Hieringer, Wolfgang (Bonn)
30. Jansen, Georg (Essen)
31. Jödicke Jamorski, Christine (Bonn)

32. Joergensen, Poul (Aarhus, Dänemark)
33. Kaupp, Martin (Würzburg)
34. Klopper, Wim (Karlsruhe)
35. Kolb, Dietmar (Kassel)
36. Kratzer, Peter (Berlin)
37. Kurth, Stefan (Berlin)
38. Kutzelnigg, Werner (Bochum)
39. Lathiotakis, Nektarios (Berlin)
40. Lechner, Ulrich (Frankfurt)
41. Legezn, Ors (Budapest)
42. Lüchow, Arne (Aachen)
43. Moritz, Gerrit (Bonn)
44. Nest, Mathias (Potsdam)
45. Noack, Reinhard (Marburg)
46. Ochsenfeld, Christian (Tübingen)
47. Paragan, Joseph (Kassel)
48. Paulus, Beate (Dresden)
49. Perlov, Alexander (München)
50. Pittalis, Stefano (Berlin)
51. Plunien, Günter (Dresden)
52. Pyykkö, Pekka (Helsinki)
53. Rao Chimnasetty, Sambasiva (Leipzig)
54. Reiher, Markus (Bonn)
55. Richter, Manuel (Dresden)
56. Rissler, Jörg (Marburg)
57. Saalfrank, Peter (Potsdam)
58. Sandratskii, Leonid (Halle)
59. Sargolzaei, Mahdi (Dresden)
60. Scott, Tony (Aachen)
61. Schindlmayr, Arno (Jülich)
62. Schneider, Reinhold (Kiel)
63. Schnurpfeil, Alexander (Siegen, Köln)
64. Soerensen, Lasse K. (Düsseldorf)
65. Springborg, Michael (Saarbrücken)
66. Stoll, Hermann (Stuttgart)
67. Van Wüllen, Christoph (Berlin)
68. Villani, Christian (Karlsruhe)
69. Wildenhues, Ralf (Bonn)
70. Wolf, Alexander (Jena)

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 20, 2005)

Monday, July 4, 2005

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

Tuesday July 5, 2005

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

Oral presentations VI

16:15 - 16:50 Arno Schindlmayr (Jülich)
Electronic structure and excitation spectra of periodic solids within first-principles many-body perturbation theory

16:50 - 17:00 Discussion

17:00 - 17:20 Martin Schütz (Regensburg)
Development of local electron corelation methods for periodic systems

17:20 - 17:25 Discussion

17:25 - 17:35* Beate Paulus (Dresden)
Development of a wavefunction-based ab-initio method for group II metals applying the method of increments

17:35 - 17:45* Alejandro Saenz (Berlin)
Ab-initio treatment of systems with translational symmetry using confined Gaussians

17:45 - 17:55* Michael Springborg (Saarbrücken)
Development and implementation of theoretical methods for dealing with functions of the quantum-mechanical operator r in extended systems

18:00 - 19:30 **Dinner**

18:00 - ... **Review panel board:** Second meeting

Oral presentations VII

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

20:05 - 20:15 Discussion

Poster session II/SPP 1145 Meeting

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

Wednesday July 6, 2005

7:00 - 9:00 **Breakfast**

9:00 - ... **Review panel board**: Third meeting (if required)

Oral presentations VIII

9:00 - 9:35 Trond Saue (Strasbourg)
Perspectives on 2- and 4-component relativistic calculations

9:35 - 9:45 Discussion

9:45 - 10:20 Claudia Filippi (Leiden)
Quantum Monte Carlo for ground and excited-state calculations

10:20 - 10:30 Discussion

10:30 - 11:00 **Coffee break**

Oral presentations IX

11:00 - 11:35 Andreas Savin (Paris)
The multi-configuration Kohn-Sham method

11:35 - 11:45 Discussion

11:45 - 12:20 Stefan Goedecker (Basel)

12:20 - 12:30 Discussion
Global minimum determination of the Born-Oppenheimer surface within density functional theory

12:30 - 14:00 **Lunch**
Departure

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

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. Hamackers, 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

6.2 Workshops

In the first financing period two workshops were organized within the SPP 1145 so far in 2004 and 2005, cf. the programmes and listings of participants given below.

During the second financing period several workshops are under consideration. A third workshop is planned by Hubert Ebert (München) and Eberhard Groß (Berlin) for spring 2006 on the tentative topic *First-principles approaches to optical and photoelectron spectra*. Another workshop organized by Andreas Görling (Erlangen) in spring 2007 is under discussion. Willem Klopper (Karlsruhe) is willing to organize a workshop on *Highly Accurate Molecular Electronic Structure Methods* on topics like R12-methods, Quantum Monte Carlo, Density Matrix Renormalization Group approaches and more in summer 2007.

6.2.1 Workshop Numerical Analysis in Quantum Chemistry (June 28 - 30, 2004, Kiel

Organizers:

- Prof. Dr. Reinhold Schneider (Kiel)
- Prof. Dr. Wolfgang Hackbusch (Leipzig)
- Prof. Dr. Bernd Hardtke (Kiel)

Number of participants: 44

homepage: http://www.numerik.uni-kiel.de/scs/

The theme of the workshop were efficient numerical methods and recent developments in numerical analysis, which have a direct relevance for problems in quantum chemistry. Topics comprised linear scaling methods for Hartree-Fock as well as Kohn-Sham approaches as well as for the evaluation of the correlation energy; density matrix evaluations; explicitly correlated wavefunction approaches (R_{12}-approaches); fast evaluation of non-local operators (Hamiltonian matrices, fast multipole exansions, ..); thin grid methods and high dimensional problems; wavelet basis sets.

6.2.2 Workshop Orbital Functionals for Exchange and Correlation: The Optimized Effective Potential and Related Methods (March 11 - 13, 2005, Berlin)

Organizers:

- Priv.-Doz. Dr. Stefan Kurth (Berlin)
- Prof. Dr. Eberhard K. U. Gross (Berlin)
- Prof. Dr. Hubert Ebert (München)

Number of participants: 72

homepage: http://www.physik.fu-berlin.de/∼ag-gross/oep-workshop/index.html

6.2.3 Programs and lists of participants of workshops 2004 - 2005

The DFG-Priority Program 1145 Modern and universal first-principles methods for many-electron systems in chemistry and physics in cooperation with the GAMM Committee Efficient numerical methods for pdes and the Christian-Albrechts-University of Kiel organises the workshop

1st Scientific Computing Seminar

Numerical Analysis in Quantum Chemistry

Christian-Albrechts-University of Kiel, Germany
June 28th to 30th, 2004.

June 2004

Su	Mo	Tu	We	Th	Fr	Sa
		1	2	3	4	5
6	7	8	9	10	11	12
13	14	15	16	17	18	19
20	21	22	23	24	25	26
27	28	29	30			

Organisers:

Reinhold Schneider (CAU Kiel), Wolfgang Hackbusch (MPI Leipzig) and Bernd Hartke (CAU Kiel)

Seminar Topics:

The seminar focuses on recent development in numerical analysis related to problems in electronic structure calculation e.g.

- Linear scaling methods for Hartree-Fock and Kohn Sham equations,,
- Linear scaling in post Hartree-Fock methods,
- density matrix methods,
- R_{12}-methods
- efficient numerical methods for non-local operators like H-matrices and fast multipol methods,
- wavelet techniques and
- sparse grid approximation for high dimensional problems,
- reaction dynamics,
- multiconfiguration time-dependent Hartree and
- reaction path/surface methods.

List of invited Speakers:

Claude Le Bris (Paris), Heinz-Jürgen Flad (MPI Leipzig), Stefan Goedecker (Basel), Michael Griebel (Bonn), Wim M. Klopper (Karlsruhe), Christian Lubich (Tübingen), Hans-Dieter Meyer (Heidelberg), Hans-Joachim Werner(Stuttgart), Harry Yserentant (Berlin)

Conference fee:

30 Euro (to be paid after arrival)

Place and Time:

The seminar will take place at the Christian-Albrechts-University in Kiel (Ludewig-Meyn-Str. 2, Seminarraum UE2). The first lecture will be given on Monday, 28th of June, 2004, at 13 h. The seminar ends on Wednesday, 30th of June, 2004.

Registration:

Please use our electronic registration form or send a letter to the local organiser.

Local organisation:

Jens Burmeister, Tel.: ++49(0)431-880-4462, Fax: ++49(0)431-880-4464, Email: jb@numerik.uni-kiel.de

We use XHTML and CSS

Announcement | Registration | Programme (Monday, Tuesday, Wednesday)

The DFG-Priority Program 1145 Modern and universal first-principles methods for many-electron systems in chemistry and physics in cooperation with the GAMM Committee Efficient numerical methods for pdes and the Christian-Albrechts-University of Kiel organises the workshop

1st Scientific Computing Seminar

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June 2004

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13	14	15	16	17	18	19
20	21	22	23	24	25	26
27	28	29	30			

Scientific programme on Monday, 28th of June, 2004

Time		Author(s) / Speaker / Title of the lecture
13.00 - 13.10	-	Opening of seminar and Monday session
13.10 - 14.10	i	Michael Griebel (Bonn): Sparse Grids for Schrödinger-type equations
14.10 - 14.40	i	Alexey Neelov (Basel, Switzerland) Convergence and performance analysis of wavelet methods for the solution of Schrödinger equation
	-	Coffee break
14.55 - 15.55	i	Harry Yserentant (Berlin): The smoothness of electronic wave functions and ways to exploit it
15.55 - 16.25	i	Wolfgang Hackbusch (Leipzig): Approximation of 1/r by sums of exponentials
	-	Coffee break
16.55 - 17.25	i	Tomasz Wesolowski (Geneva, Switzerland): Partitioning the electron density as a formal route towards linear-scaling
17.25 - 17.45	i	Thomas Kastl (Zürich, Switzerland) Hierarchical matrices in density functional theory
17.45 - 18.15	i	Lars Grasedyck (Leipzig): Existence and computation of low Kronecker-rank approximations for large linear systems of tensor product structure
18.15 - 18.45	i	A. K. Prykarpatsky (Krakow, Poland): Quantum Holonomic Computing, Grassmannian Manifolds and Dual Momentum Mappings
	-	End of Monday session

We use XHTML and CSS

The DFG-Priority Program 1145 Modern and universal first-principles methods for many-electron systems in chemistry and physics in cooperation with the GAMM Committee Efficient numerical methods for pdes and the Christian-Albrechts-University of Kiel organises the workshop

1st Scientific Computing Seminar

Numerical Analysis in Quantum Chemistry

Christian-Albrechts-University of Kiel, Germany
June 28th to 30th, 2004.

June 2004

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6	7	8	9	10	11	12
13	14	15	16	17	18	19
20	21	22	23	24	25	26
27	28	29	30			

Scientific programme on Tuesday, 29th of June, 2004

Time		Author(s) / **Speaker** / Title of the lecture
	-	Opening of Tuesday session
8.30 - 9.30	i	Stefan Goedecker (Basel, Switzerland): Achieving linear scaling in electronic structure calculations and atomistic simulations
9.30 - 10.15	i	Heinz-JürgenFlad (Leipzig): Wavelet Approach to Jellium-Type Models
	-	Coffee break
10.45 - 11.45	i	Wim M. Klopper (Karlsruhe): Convergence behaviour and convergence acceleration of molecular electronic wave functions
11.45 - 12.30	i	Bastiaan J. Braams (Atlanta, USA): The reduced density matrix method for electronic structure calculations, and a new approach for fitting a potential energy surface
	-	Lunch
14.00 - 15.00	i	Claude Le Bris (Paris, France): Numerical analysis for computational chemistry: an overview of years of efforts
15.00 - 15.30	i	Dietmar Kolb (Kassel): Minimax Relativistic for Molecules
	-	Coffee break
15.50 - 16.50	i	Hans-Joachim Werner (Stuttgart): Local correlation methods combined with density fitting approximations
16.50 - 17.20	i	Arno Schindlmayr (Jülich) Efficient Numerical Implementation of the GW Approximation
	-	Coffee break
17.35 - 18.05	i	Peter Koval, Stephan Fritzsche (Kassel): Implicit summation techniques in atomic physics
18.05 - 18.35	i	V. Popescu, H. Ebert, R. Zeller, P. H. Dederichs (München) A fully relativistic implementation of the screened Korringa-Kohn-Rostoker Green's Function method
	-	End of Tuesday session

The DFG-Priority Program 1145 Modern and universal first-principles methods for many-electron systems in chemistry and physics in cooperation with the GAMM Committee Efficient numerical methods for pdes and the Christian-Albrechts-University of Kiel organises the workshop

1st Scientific Computing Seminar

Numerical Analysis in Quantum Chemistry

Christian-Albrechts-University of Kiel, Germany
June 28th to 30th, 2004.

June 2004

Su	Mo	Tu	We	Th	Fr	Sa
		1	2	3	4	5
6	7	8	9	10	11	12
13	14	15	16	17	18	19
20	21	22	23	24	25	26
27	28	29	30			

Scientific programme on Wednesday, 30th of June, 2004

Time		Author(s) / **Speaker** / Title of the lecture
	-	Opening of Wednesday session
8.30 - 9.30	i	Christian Lubich (Tübingen) Variational splitting integrators for quantum molecular dynamics
9.30 - 10.00	i	Illia Horenko, Burkhard Schmidt, Christof Schütte, Martin Weiser (Berlin) Fully Adaptive Propagators in Molecular Dynamics
	-	Coffee break
10.30 - 11.30	i	Hans-Dieter Meyer (Heidelberg): Multiconfiguration time-dependent Hartree (MCTDH): An efficient method for propagating multi-dimensional wavepackets and density operators
11.30 -12.00	i	Caroline Lasser (München), Stefan Teufel (Warwick, UK) A rigorous surface hopping algorithm
12.00 -12.30	i	Andrew Torda (Hamburg): Protein force fields based on empiricism, optimism and optimisation
	-	End of Wednesday session and seminar

First Scientific Computing Seminar
June 28 - 30, 2004, Kiel

Participants:

1. Bastian J. Braams (Atlanta)
2. Jens Burmeister (Kiel)
3. Monica Ciantelli-Haynes (Mönchengladbach)
4. Sambasiva Rao Chinnamsetty (Leipzig)
5. Priv.-Doz. Dr. Birgit Faermann (Kiel)
6. Kim Feldhoff (Karlsruhe)
7. Dr. Heinz-Jürgen Flad (Leipzig)
8. Dr. Stefan Funken (Berlin)
9. Prof. Dr. Stefan Goedecker (Basel)
10. Dr. Vasile Gradinaru (Tübingen)
11. Dr. Lars Grasedyck (Leipzig)
12. Prof. Dr. Michael Griebel, Bonn
13. Prof. Dr. Wolfgang Hackbusch (Leipzig)
14. Jan Hamaekers (Bonn)
15. Prof. Dr. Bernd Hartke (Kiel)
16. Dr. Wolfgang Hieringer (Bonn)
17. Thomas Kastl (Zürich)
18. Prof. Dr. Willem Klopper, Karlsruhe
19. Prof. Dr. Dietmar Kolb (Kassel)
20. Ognyan Kounchev (Duisburg)
21. Peter Koval (Kassel)
22. Caroline Lasser (München)
23. Claude Le Bris (Marne La Vallee)
24. Prof. Dr. Christian Lubich (Tübingen)
25. Prof. Dr. Arne Lüchow (Aachen)
26. Dr. Hongjun Luo (Kassel)
27. Dr. Hans-Dieter Meyer (Heidelberg)
28. Wolfgang Müller (Karlsruhe)
29. Alexey Neelov (Basel)
30. Dr. Mathias Nest (Postdam)
31. Dr. Voicu Popscu (München)
32. Roman Reviakine (Würzburg)
33. Dr. Arno Schindlmayer (Jülich)
34. Priv.-Doz. Dr. Burkhard Schmidt (Berlin-Dahlem)
35. Prof. Dr. R. Schneider, Chemnitz
36. Dr. Tony Scott (Aachen)
37. Lasse Kragh Sorensen (Düsseldorf)

38. Dr. Andrew Torda (Hamburg)
39. Toralf Weber (Kiel)
40. Dr. Gerrit Welper (Aachen)
41. Prof. Dr. Hans-Joachim Werner (Stuttgart)
42. Tomosz Wesolowski (Genf)
43. Ralf Wildenhues (Bonn)
44. Prof. Dr. Harry Yserentant (Berlin)

Report on the Workshop

Orbital Functionals for Exchange and Correlation: The Optimized Effective Potential and Related Methods

March 11-13, 2005, Berlin, Germany

This workshop has been organized by S. Kurth and E.K.U. Gross (both from the Freie Universität Berlin) and H. Ebert (Ludwig-Maximilians-Universität München). It was funded mainly through the priority program SPP 1145 "First-Principles Methods" of the DFG and the EU Network of Excellence NANOQUANTA. The scientific program covered 31 invited and 4 contributed talks and was attended by 72 participants.

The focus of the workshop was on the latest theoretical developments of orbital functionals within density-functional theory and on many-body perturbation theory approaches like the GW method. Other topics included dynamic mean field theory, reduced density-matrix functional theory and density functional theory for superconductors.

New developments were reported on the construction of better orbital functionals for electron correlation. Several groups have studied orbital functionals obtained from second order perturbation theory, from RPA or GW-type methods or from variational functionals of the many-body Green function. These developments are stimulated by an interest in calculating optical properties of solids and molecules which require better response functions based on the exchange-correlation kernel of time-dependent density functional theory. Several groups at the workshop presented ways to develop density-functional procedures which are aimed to compete in accuracy with many-body methods based on the Bethe-Salpeter equation while reducing the computational effort considerably.

In several talks, results obtained with self-interaction corrected functionals were presented. The optimized effective potential method has been studied for the (static and dynamic) electrical response of finite systems and in a relativistic framework for the description of magnetic solids.

A different line of research presented at the workshop aims at an ab-initio description of strongly correlated materials. In this context, dynamic mean field theory was discussed in several talks and a reduced density matrix functional method based on natural orbitals and occupation numbers was presented.

Details of the program and many of the talks can be found at the workshop webpage at http://www.physik.fu-berlin.de/∼ag-gross/oep-workshop/index.html

Program of OEP Workshop, March 11-13, 2005, Berlin

Time	Friday	Saturday	Sunday
9.00-9.30		**H. Eschrig** Orbital Polarization in the Kohn-Sham-Dirac Theory	**L. Reining** Many-Body Perturbation Theory using the Density-Functional concept: a successful combination!
9.30-10.00		**S. Kurth** Optimized Effective Potentials in Current-Density-Functional Theory	**A. Rubio** Optical and ground state properties of solids within a GW-based OEP scheme
10.00-10.30		**M. Kaupp** The quest for inclusion of nondynamical electron correlation in OEP calculations	**F. Bechstedt** GW approximation: One- and two-particle excitations in solids and molecules
10.30-11.00		**Coffee Break**	**Coffee Break**
11.00-11.30		**R. Godby** Including orbital effects in exchange and correlation through generalized Kohn-Sham and GW approaches	**E. Engel** Including orbital effects in perturbation theory: Asymptotic properties of correlation potential for finite systems
11.30-12.00		**P. Rinke** Combining quasiparticle energy calculations with exact-exchange density-functional theory	**X. Gonze** Orbital- and energy-dependent exchange-correlation functionals : molecular dissociation and band gap energy
12.00-12.30		**A. Schindlmayr** Surface Contributions to the Self-Energy for Slab and Supercell Geometries	**N. Lathiotakis** Electronic correlation in periodic systems using reduced density matrix functional theory
12.30-13.30		**Lunch**	**Lunch**
13.30-14.00	**A. Görling** Exact-exchange methods as examples of density-functional approaches with orbital-dependent functionals	**Lunch**	**Lunch**
14.00-14.30	**S. Kümmel** Optimized effective potential and the electrical response of finite systems	**K. Tsemekhman** Self-Consistent implementation of SIC DFT and of the exact exchange functionals in plane-wave DFT*	**U. von Barth** Successively better and conserving response function within time-dependent density-functional theory obtained from variational many-body theory
14.30-15.00	**C. Proetto** Novel properties of the Kohn-Sham exchange potential for open systems*	**M. Lüders** Single-site self-interaction correction in the KKR-CPA*	**N.E. Dahlen** Orbital functionals derived from variational functionals of the Green function
15.00-15.30	**H. Ebert** Relativistic Optimized Potential Method for magnetic solids	**S. Biermann** A dynamical mean field view on the electronic structure of correlated materials: "LDA+DMFT" and beyond	**M. Seidl** An XC-functional with exact exchange, using the ideas of strictly correlated electrons and attractive-electron clusters
15.30-16.00	**H. Akai** OEP method in RPA level and its applications	**A. Lichtenstein** Orbital polarization in correlated electron systems	**N. Gidopoulos** Beyond the Born-Oppenheimer/adiabatic approximation in terms of an OEP
16.00-16.30	**Coffee Break**	**Coffee Break**	**Departure**
16.30-17.00	**W. Temmerman** SIC-LSD description of rare earths and actinides	**A. Eguiluz** The dynamical density-response function of transition-metal oxides	
17.00-17.30	**Z. Szotek** SIC-LSD description of spintronics materials	**M. van Schilfgaarde** Quasiparticle self-consistent GW approximation	
17.30-18.00	**A. Floris** Density functional theory for superconductors: Applications to MgB2 and solids under pressure	**A. Ernst** GW approximation in the multiple-scattering theory	
18.00-18.20	**S. Sharma** Exact exchange within the FP-LAPW method	**G. Kresse** Performance of hybrid density functional methods, screened exchange and EXX-OEP methods in the PAW approach	
18.20-18.40	**J.K. Dewhurst** Exact exchange within the FP-LAPW method	**I. Grabowski** Orbital dependent correlation potentials in ab initio density functional theory	

List of Participants of the Workshop

Orbital Functionals for Exchange and Correlation: The Optimized Effective Potential and Related Methods

March 11-13, 2005, Berlin, Germany

	Name	Institution	Country
1	Hisazumi Akai	Osaka University	Japan
2	Claudia Ambrosch-Draxl	Universität Graz	Austria
3	Heiko Appel	Freie Universität Berlin	Germany
4	Alexei Arbouznikov	Universität Würzburg	Germany
5	Friedhelm Bechstedt	Universität Jena	Germany
6	Silke Biermann	École Polytechnique, Palaiseau	France
7	Nuño Carneiro	York University	United Kingdom
8	Alberto Castro	Freie Universität Berlin	Germany
9	Nils-Erik Dahlen	Rijksuniversiteit Groningen	The Netherlands
10	Kay Dewhurst	Universität Graz	Austria
11	Hubert Ebert	LMU München	Germany
12	Adolfo Eguiluz	University of Tennessee, Knoxville	USA
13	Eberhard Engel	Universität Frankfurt	Germany
14	Arthur Ernst	MPI für Mikrostrukturphysik Halle	Germany
15	Helmut Eschrig	IFW Dresden	Germany
16	Volker Eyert	Universität Augsburg	Germany
17	Heinz-Jürgen Flad	MPI für Mathematik in den Naturwissenschaften, Leipzig	Germany
18	Andrea Floris	Freie Universität Berlin	Germany
19	Frank Fuchs	Universität Jena	Germany
20	Matteo Gatti	École Polytechnique, Palaiseau	France
21	René Gaudoin	Donostia International Physics Center, San Sebastian	Spain
22	Nikitas Gidopoulos	Rutherford-Appleton Lab Oxford	United Kingdom
23	Henning Glawe	Freie Universität Berlin	Germany
24	Rex Godby	York University	United Kingdom
25	Xavier Gonze	University Louvain-la-Neuve	Belgium
26	Andreas Görling	Universität Erlangen	Germany
27	Irek Grabowski	Torun University	Poland
28	Eberhard Gross	Freie Universität Berlin	Germany
29	Myrta Grüning	Donostia International Physics Center, San Sebastian	Spain
30	Nicole Helbig	Freie Universität Berlin	Germany
31	Maria Hellgren	Lund University	Sweden
32	Andreas Hermann	Universität Jena	Germany
33	Hong Jiang	Universität Frankfurt	Germany
34	Martin Kaupp	Universität Würzburg	Germany
35	Diemo Ködderitzsch	LMU München	Germany
36	Georg Kresse	Universität Wien	Austria
37	Stephan Kümmel	MPI for the Physics of Complex Systems, Dresden	Germany
38	Stefan Kurth	Freie Universität Berlin	Germany
39	Nektarios Lathiotakis	Freie Universität Berlin	Germany
40	Alexander Lichtenstein	Universität Hamburg	Germany
41	Martin Lüders	Daresbury Laboratories, Warrington	United Kingdom
42	Michael Mundt	MPI for the Physics of Complex Systems, Dresden	Germany
43	Anna Okopinska	University of Kielce	Poland
44	Giovanni Onida	University of Milano	Italy
45	Stefano Pittalis	Freie Universität Berlin	Germany
46	Yann Pouillon	University Louvain-la-Neuve	Belgium
47	César Proetto	Centro Atómica Bariloche	Argentina
48	Virginie Quequet	École Polytechnique, Palaiseau	France
49	Lucia Reining	École Polytechnique, Palaiseau	France
50	Patrick Rinke	Fritz-Haber Institut Berlin	Germany
51	Carlo Rozzi	Freie Universität Berlin	Germany
52	Angel Rubio	Donostia International Physics Center, San Sebastian	Spain
53	Stephan Sagmeister	Universität Graz	Austria
54	Arno Schindlmayr	Forschungszentrum Jülich	Germany
55	Reinhold Schneider	Universität Kiel	Germany
56	Michael Seidl	Universität Regensburg	Germany
57	Sangeeta Sharma	Universität Graz	Austria
58	Martin Stankovski	York University	United Kingdom
59	Gianluca Stefanucci	Lund University	Sweden
60	Zdizislawa Szotek	Daresbury Laboratories, Warrington	United Kingdom
61	Walter Temmerman	Daresbury Laboratories, Warrington	United Kingdom
62	Kiril Tsemekhman	University of Washington, Seattle	USA
63	Robert van Leeuwen	Rijksuniversiteit Groningen	The Netherlands
64	Mark van Schilfgaarde	Arizona State University, Tempe	USA
65	Ulf von Barth	Lund University	Sweden
66	Jan Werschnik	Freie Universität Berlin	Germany
67	Bogdan Yavorski	Universität Halle	Germany
68	Angelica Zacarias	Freie Universität Berlin	Germany
69	Peter Zahn	Universität Halle	Germany
70	Hand Zenia	Daresbury Laboratories, Warrington	United Kingdom
71	Vladen Zhukov	Donostia International Physics Center, San Sebastian	Spain
72	Paul Ziesche	MPI for the Physics of Complex Systems, Dresden	Germany

6.3 Guests and visits to other laboratories

In the first financing period of the SPP 1145 each project was assigned 1.500,– Euro for travel costs and 1.100,– Euro for inviting guests.

Table 1: Guest scientists invited to research groups of the SPP 1145. Only guests in direct connection with ongoing SPP research projects or financed by the SPP 1145 are listed. (duration of visit: d=day(s), w=week(s), m=month(s), s=several short visits, n=no information given)

name	home institution/city	host in SPP 1145/city	duration of visit	topic/purpose of visit
M. Albrecht	Siegen	Gross/Berlin	7d (2004)	collaboration
M. Albrecht	Siegen	Dolg/Cologne	1d (2004)	seminar
	seminar title:			
J. Anton	Kassel	Engel/Frankfurt	1d ()	seminar
	seminar title: *Relativistische Dichte-Funktional-Rechnungen für kleine Moleküle und Cluster*			
T. Auth	Jülich	Engel/Frankfurt	2d (2004)	seminar
	seminar title: *Effective curvature-elastic constants for membrane-polymer systems*			
V. Balashov	Moscow (Russia)	Fritzsche/Kassel	2d (2005)	collaboration and seminar
	seminar title: *Kinetics of interactions of highly-charged ions with matter*			
M.S.S. Brooks	Uppsala (Sweden)	Eschrig/Dresden	2d (2004)	seminar
	seminar title: *Theory of spin and orbital magnetization densities with screened exchange interactions*			
C. Dong	Lanzhou (V.R. China)	Fritzsche/Kassel	2m (2005)	common program development
A. Dreuw	Frankfurt	Stoll/Stuttgart	1d ()	seminar
	seminar title: *Charge-transfer states in TD-DFT*			
R. Evarestov	St. Petersburg (Russia)	Schütz/Regensburg	2d ()	seminar
	seminar title: *Quantum chemical modelling of crystalline surfaces*			
F. Furche	Essen	Stoll/Stuttgart	1d ()	seminar
	seminar title: *Time-dependent density functional methods*			
G. Gaigalas	Vilnius (Lithuania)	Fritzsche/Kassel	2m (2005)	common program development
	seminar title: *topic: unit tensors in atomic shell models*			
P. M. W. Gill	Nottingham (UK)	Dolg/Cologne	2d (2004)	Hartree-Fock-Wigner theory
	seminar title: *A new type of functional for density functional theory*			
A. Hesselmann	Essen	Stoll/Stuttgart	1d ()	seminar
	seminar title: *Intermolecular DFT-SAPT approach*			
M. Inal	Tlemcen (Algerien)	Fritzsche/Kassel	2m (2004)	density matrix theory in atomic collisions
	seminar title: *topic: ?*			

Table 1: Guest scientists, continued.

name	home institution/city	host in SPP 1145/city	duration of visit	topic/purpose of visit
H. J. Aa. Jensen	Odense (Denmark)	Fleig/Dsseldorf	5d (2005)	seminar and collaboration
	seminar title: *An MCSCF-DFT Hybrid Approach*			
M. Kallay	Budapest (Hungary)	Gauss/Mainz	1m ()	CC methods with approximate higher excitations
M. Kallay	Mainz	Fleig/Dsseldorf	1d (2004)	seminar
	seminar title: *String-Based Implementation of Quantum Chemical Methods*			
T. Kotani	Osaka (Japan)	Schindlmayer/Jülich	4w (2004)	common program development
S. Kuemmel	Dresden	Eschrig/Dresden	n	seminar
	seminar title: *Orbitalfunktionale in der Dichtefunktionaltheorie*			
S. Kurth	Berlin	Saalfrank/Potsdam	1d ()	seminar
	seminar title: *topic: TD-DFT*			
V. G. Malkin	Bratislava (Slovakia)	Kaupp/Würzburg	s ()	DFT and NMR/ESR
O. L. Malkina	Bratislava (Slovakia)	Kaupp/Würzburg	s ()	DFT and NMR/ESR
L. Maschio	Torino (Italy)	Schütz/Regensburg	3m ()	density fitting CRYSCOR
J. Olsen	Odense (Denmark)	Fleig/Dsseldorf	4d ()	seminar and collaboration
	seminar title: *Coupled Cluster to the Limit*			
B. Paulus	Dresden	Eschrig/Dresden	n	seminar
	seminar title: *Ab initio correlation treatment of solid mercury*			
S. Patchkovskii	NRC Canada	Eschrig/Dresden	1m ()	collaboration on current density functional theory and NMR calculations
M. Pederson		Eschrig/Dresden	1w (2004)	seminar
	seminar title: *Molecular magnets*			
K. Rashid	Islamabad (Pakistan)	Fricke/Kassel	4w ()	calculations on heavy diatomics
R. M. Pitzer	Columbus (USA)	Dolg/Cologne	2d (2005)	seminar
	seminar title: *Excited States of Some Lanthanide Systems*			
P. Pyykkoe	Helsinki (Finland)	Eschrig/Dresden	3d (2004)	seminar
	seminar title: *Towards valence-shell QED in quantum chemistry*			

Table 1: Guest scientists, continued.

name	home institution/city	host in SPP 1145/city	duration of visit	topic/purpose of visit
L. Seijo	Madrid (Spain)	Dolg/Cologne	2d (2005)	seminar
	seminar title: *Mosaico: a parallel, linear-scaling building-block and embedding method based on localized orbitals and orbital-specific basis sets*			
T. Weber	Kiel	Flad/Leipzig	6d (2004)	collaboration
K. Yabana	Tsukuba (Japan)	Gross/Berlin	3d ()	seminar
	seminar title: *topic: time-dependent DFT*			
I. Zilberberg	Novosibirsk (Russia)	Kaupp/Würzburg	4d	seminar
	seminar title: *Analysis of spin contamination in DFT calculations using paired orbital concepts.*			

Table 2: Visits of researchers of the SPP 1145 to other research groups and/or conferences/workshops. Excluded from this list are the participation at the SPP 1145 symposia in 2003/2004 as well as the SPP 1145 workshops in 2004/2005 (for these please refer to the lists of participants as well as the programs listed above in this report). Poster contributions on conferences and workshops are not mentioned here.

name	city	visited institution/city	duration of visit	topic
J. Anton	Kassel	Mühlheim	3d (2005)	REHE conference
J. Anton	Kassel	P. Schwerdtfeger/Auckland	1m (2004)	collaboration on relativistic DFT
H. Ebert	München	Dresden	3d ()	workshop Strong Correlations and ARPES
	seminar title: *A fully relativistic implementation of the screened Korringa-Kohn-Rostoker Green's Function method*			
H. Ebert	München	Mannheim	3d ()	workshop Excited-state Properties of Solids
	seminar title: *Calculation of photo-emission spectra on the basis of a combination of the KKR method and the DMFT*			
H. Ebert	München	Hamburg	2d ()	Hands on DMFT Course
	seminar title: *LDA+DMFT in the KKR-scheme*			
H. Ebert	München	Manchester (UK)	3d ()	Local-SIC-meeting
	seminar title: *The OPM applied to magnetic solids - aspects and present status*			
H. Ebert	München	Berlin	3d (2005)	DPG-Früjahrstagung
	seminar title: *Multiple scattering formalism for correlated systems: A KKR+DMFT approach*			
H. Ebert	München	Poznan (Poland)	3d (2005)	Conference Physics of Magnetism
	seminar title: *Relativistic and correlation effects in magnetic solids*			
E. Engel	Frankfurt	Lyon	5d (2005)	CECAM workshop on van der Waals forces and DFT
	seminar title: *Description of van der Waals Forces by Implicit Density Functionals*			
T. Fleig	Düsseldorf	Sønderborg (Denmark)	4d (2005)	Conference Response Theory and Molecular Properties
T. Fleig	Düsseldorf	Jülich	1d (2004)	Introduction to new supercomputer JUMP
T. Fleig	Düsseldorf	Suhl	5d (2004)	Symposium for Theoretical Chemistry
T. Fleig	Düsseldorf	L. Visscher/Amsterdam (Netherlands)	2d (2005)	collaboration on CI, CC
R. Fondermann	Köln	Sostrup (Denmark)	12d (2004)	12th Sostrup summer school for quantum chemistry and molecular properties
R. Fondermann	Köln	Karlsruhe	4d (2005)	Nanoscience workshop: Computational Tools for Molecules, Clusters and Nanostructures
B. Fricke	Kassel	P. Schwerdtfeger/Auckland	1m (2004)	collaboration on rel. DFT
C. Friedrich	Jülich	Acquafredda di Maratea (Italy)	5d (2004)	workshop Theory and Modeling of Electronic Excitations in Nanoscience
J. Gauss	Mainz	P. Szalay/Budapest (Hungary)	1w (2005)	collaboration CC for open shell systems
	seminar title: *New developments for the electron-correlated calculation of magnetic properties*			

Table 2: Visits of SPP 1145 researchers, continued.

name	city	visited institution/city	duration of visit	topic
E. Goll	Stuttgart	Lyon (Frankreich)	4d (2005)	CECAM workshop on Van der Waals forces and DFT
E. Goll	Stuttgart	Karlsruhe	3d (2005)	Nanoscience workshop
E. Goll	Stuttgart	Hirschegg (Austria)	3d (2005)	Electron correlation workshop
M. Griebel	Bonn	Berlin	3d ()	Workshop Numerische Verfahren zur Lösung der Schrödingergleichung
	seminar title: *Sparse grid methods for the Schrödinger equation*			
J. Hamaekers	Bonn	Berlin	3d ()	Workshop Numerische Verfahren zur Lösung der Schrödingergleichung
M. Hanrath	Köln	Karlsruhe	4d (2005)	Nanoscience workshop: Computational Tools for Molecules, Clusters and Nanostructures
M. Heckert	Mainz	P. Szalay/Budapest (Hungary)	3w (2005)	CC for open shell systems
D. Koedderitzsch	München	Hamburg	3d ()	Hands on DMFT course
D. Koedderitzsch	München	Manchester (UK)	3d ()	Local-SIC-meeting
S. Kurth	Berlin	Maratea (Italy)	5d (2004)	Workshop on DFT
	seminar title: *Orbital Functionals in Current-DFT*			
N. Lathiotakis	Berlin	Manchester (UK)	4d ()	L-SIC mmeting
	seminar title: *Application of reduced density matrix functional theory to periodic systems*			
N. Lathiotakis	Berlin	M. Albrecht/Siegen	4d (2004)	collaboration density matrix theory
N. Lathiotakis	Berlin	M. Albrecht/Siegen	9d (2005)	collaboration density matrix theory
M. Nest	Potsdam	Zeuthen	n (2005)	workshop Ultrafast Dynamics
M. Nest	Postdam	A. Scrinzi/Wien (Austria)		
J. Minar	München	Daresbury (UK)	3d (2004)	CCP9 Workshop
G. Moritz	Bonn	Suhl	5d (2004)	Symposium for Theoretical Chemistry
M. Reiher	Jena	Mühlheim	5d (2005)	REHE conference
	seminar title: *Infinite-Order Douglas-Kroll-Hess Theory*			
K. Rykhlinskaya	Kassel	Düsseldorf	3d (2005)	REHE conference
A. Schindlmayr	Jülich	Acquafredda di Maratea (Italy)	5d ()	workshop Theory and Modeling of Electronic Excitations in Nanoscience

Table 2: Visits of SPP 1145 researchers, continued.

name	city	visited institution/city	duration of visit	topic
A. Schindlmayr	Jülich	T. Miyake/Tokyo (Japan)	4w ()	collaboration on maximum localized Wannier functions
A. Perlov	München	Hamburg	2d (2004)	collaboration and seminar
	seminar title: *?*			
S. Pittalis	Berlin	Acquafredda di Maratea (Italy)	5d (2004)	workshop Theory and Modeling of Electronic Excitations in Nanoscience
S. Pittalis	Berlin	Berlin	2d (2005)	NANQUANTA Workshop
	seminar title: *Optimized Effective Potentials in Current-DFT*			
H. Stoll	Stuttgart	Karlsruhe	3d (2005)	Nanoscience workshop: Computational Tools for Molecules, Clusters and Nanostructures
H. Stoll	Stuttgart	Hirschegg (Austria)	3d (2005)	Electron correlation workshop
M. Schütz	Stuttgart	Torino	5d (2004)	collaboration on CRYSTAL package
	seminar title:			
M. Schütz	Regensburg	Torino	-	workshop on Local Correlation Methods: from molecules to crystals
	seminar title: *Local correlation methods with density fitting*			
D. Usvyat	Stuttgart	Torino	5d (2004)	workshop on Local Correlation Methods: from molecules to crystals
R. Wildenhues	Bonn	Oberwolfach	5d (2004)	Conference Wavelet and Multiscale Methods
R. Wildenhues	Bonn	Berlin	3d ()	Workshop Numerische Verfahren zur Lösung der Schrödingergleichung
R. Wildenhues	Bonn	Canberra (Australia)	4d ()	Workshop on high-dimensional approximation
	seminar title: *Separable approximation for the Schr"odinger equation*			Lösung der Schrödingergleichung
A. Wolf	Jena	Mühlheim	5d (2005)	REHE conference
A. Wolf	Bonn	Suhl	5d (2004)	Symposium for Theoretical Chemistry