1 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. *Multireference Configuration Interaction Treatment of Excited-State Electron Correlation in Periodic Systems: the Band Structure of trans-Polyacetylene*, V. Bezugly, U. Birkenheuer, Chem. Phys. Lett. 399, 57 (2004).
17. *Localization of Wannier Functions for Entangled Energy Bands*, U. Birkenheuer, D. Izotov, Phys. Rev. B 71, 125115 (2005).
18. *A simplified method for the computation of correlation effects on the band structure of semiconductors*, U. Birkenheuer, P. Fulde, H. Stoll, Theor. Chem. Acc., submitted (2005).
19. *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).
20. *Coupled-Cluster Methods including Non-Iterative Corrections for Quadruple Excitations*, Y. Bomble, J.F. Stanton, M. Kallay, J. Gauss, J. Chem. Phys., accepted (2005).
21. *Approximation of $1/x$ by exponential sums in $[1, \infty)$*, D. Braess and W. Hackbusch, IMA J. Numer. Anal. accepted (2005).
22. *Sparse grids*, H.-J. Bungartz, M. Griebel. *Acta Numerica*, 13:1–123 (2004).
23. *Ab initio Green's Function Formalism for Band Structures*, C. Buth, U. Birkenheuer, M. Albrecht, P. Fulde, Phys. Rev. B, submitted (2005).
24. *Induced magnetic fields in aromatic annulenes*, C. Corminboeuf, Th. Heine, G. Seifert, P. Schleyer, J. Weber, Phys. Chem. Chem. Phys. 6, 273 (2004).
25. *Monte Carlo for the first dissociation energies of transition metal carbonyls*, C. Diedrich, A. Lüchow, S. Grimme, J. Chem. Phys. 122, 21101 (2005).
26. *Exchange-correlation and QED effects from a density functional based level shift approach*, E. Engel, U. Lechner, Chem. Phys. 311, 209 (2005).
27. *Solubility of the OPM integral equation for finite systems*, E. Engel, H. Jiang, A. Facco Bonetti, Phys. Rev. A., submitted (2005).
28. *Second order correlation potential of atoms in cavity*, E. Engel, H. Jiang, J. Chem. Phys., submitted (2005).
29. *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).
30. *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).
31. *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).

32. *Molecular results for Hartree-Fock-Wigner theory*, R. Fondermann, M. Hanrath, M. Dolg, D. O'Neill, Chem. Phys. Lett., submitted (2005).
33. *Coupling of short-range GGA with long-range coupled-cluster methods*, E. Goll, H.-J. Werner, H. Stoll, submitted (2005).
34. *An Exponential Multi-Reference Wavefunction Ansatz*, M. Hanrath, J. Chem. Phys., in press (2005).
35. *Equilibrium Geometries based on Coupled-Cluster Calculations involving Quadruple Excitations*, M. Heckert, M. Kallay, J. Gauss, Mol. Phys., accepted (2005).
36. *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).
37. *The magnetic shielding function of molecules and pi electron delocalization*, Th. Heine, C. Corminboeuf, G. Seifert, Chem. Rev., in press (2005).
38. *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).
39. *Analytic Second Derivatives for General Coupled-Cluster and Configuration-Interaction Models*, M. Kallay and J. Gauss, J. Chem. Phys 120, 6841 (2004).
40. *Calculation of Excited-State Properties using General Coupled-Cluster and Configuration-Interaction Models*, M. Kallay and J. Gauss, J. Chem. Phys. 121, 9257 (2004).
41. *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).
42. *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).
43. *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).
44. *Open shells in reduced-density-matrix-functional theory*, N.N. Lathiotakis, N. Helbig, E.K.U. Gross, Phys. Rev. A, Rapid Comm., submitted (2005).
45. *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).
46. *Exact-exchange density-functional calculations for noble-gas solids*, R.J. Magyar, A. Fleszar, E.K.U. Gross, Phys. Rev. B 69, 045111 (2004).
47. *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).
48. *The induced magnetic field in cyclic molecules*, G. Merino, Th. Heine, G. Seifert, Chemistry - A European Journal 10, 4367 (2004).
49. *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)

50. *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)
51. *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.
52. *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).
53. *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).
54. *Relativistic DMRG calculations on the curve crossing of cesium hydride*, G. Moritz, A. Wolf, M. Reiher, J. Chem. Phys., submitted (2005).
55. *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).
56. *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).
57. *Correlated many electron dynamics: Application to inelastic electron scattering at a metal film*, M. Nest and T. Klamroth, Phys. Rev. A, in press (2005).
58. *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).
59. *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).
60. *Exact decoupling of the Dirac Hamiltonian. I. General Theory*, M. Reiher, A. Wolf, J. Chem. Phys. 121, 2037 (2004).
61. *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).
62. *Laser-driven electron dynamics at interfaces*, P. Saalfrank, T. Klamroth, C. Huber, and P. Krause, Isr. J. Chem. 45, 205 (2005).
63. *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).
64. *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).
65. *Northogonal ultralocalized functions and fitted Wannier functions for local correlation methods for solids*, D. Usvyat, M. Schütz, Theor. Chem. Acc., in press (2005).

66. *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).
67. *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).