

# 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 or by scientists financed by the SPP 1145 during the years 2005 - 2007, roughly corresponding to the second financing period. Other publications on topics relevant to the SPP 1145, but not being a direct outcome of the SPP 1145 are not listed.<sup>1</sup>

1. *Implicit infinite lattice summations for real space ab initio correlation methods*, M. Albrecht, *Theor. Chem. Acc.* 114 (2005) 265.
2. *Towards a frequency independent incremental ab initio scheme for the self energy*, M. Albrecht, *Theor. Chem. Acc.* 116 (2006) 486.
3. *Tailoring the induced magnetism in carbon-based and non-traditional inorganic nano-materials*, A. N. Andriotis, R. M. Sheetz, N. N. Lathiotakis, M. Menon, *Int. J. of Nanotechnology* (2007) accepted.
4. *Rydberg states with quantum Monte Carlo*. A. Bande, A. Lüchow, F. Della Sala, A. Görling, *J. Chem. Phys.* 124 (2006) 114114.
5. *A simplified method for the computation of correlation effects on the band structure of semiconductors*, U. Birkenheuer, P. Fulde, H. Stoll, *Theor. Chem. Acc.* 116 (2006) 398.
6. *Localization of Wannier functions for entangled energy bands*, U. Birkenheuer, D. Izotov, *Phys. Rev. B* 71 (2005) 125116.
7. *Spectral Function of Ferromagnetic 3d Metals: A Self-Consistent LSDA+DMFT Approach Combined with the One-Step Model of Photoemission*, J. Braun, J. Minár, H. Ebert, M. I. Katsnelson, A. I. Lichtenstein, *Phys. Rev. Lett.* 97 (2006) 227601.
8. *Ab initio Greens function formalism for band structures*, C. Buth, U. Birkenheuer, M. Albrecht, P. Fulde, *Phys. Rev. B* 72 (2005) 195107.
9. *Influence of correlation effects on the magneto-optical properties of the half-metallic ferromagnet NiMnSb*, S. Chadov, J. Minár, H. Ebert, A. Perlov, L. Chioncel, M. I. Katsnelson, A. I. Lichtenstein, *Phys. Rev. B* 74 (2006) 140411(R).
10. *High-Accuracy Computation of Reaction Barriers in Enzymes*, F. Claeysens, J. N. Harvey, F. R. Manby, R. A. Mata, A. J. Mulholland, K. E. Ranaghan, M. Schütz, S. Thiel, W. Thiel, H.-J. Werner, *Angew. Chem.* 118 (2006) 7010.
11. *Generalized Hybrid Orbitals in the FA-ADMA Method*, S. Eckard, T. E. Exner, *Z. Phys. Chem.* 220(7) (2006) 927.
12. *Solubility of the OPM integral equation for finite systems*, E. Engel, H. Jiang, A. Facco Bonetti, *Phys. Rev. A* 72 (2005) 052503.
13. *Orbital-dependent representation of the correlation energy functional: Properties of second order Kohn-Sham perturbation expansion*, E. Engel, H. Jiang, *Int. J. Quantum Chem.* 106 (2006) 3242.

---

<sup>1</sup>The relevant publications of M. Albrecht, U. Birkenheuer and M. Reiher have been selected by the SPP 1145 coordinator from the publication lists of these authors available through Web-of-Science.

14. *Orbital polarization in the Kohn-Sham-Dirac theory*, H. Eschrig, M. Sargolzaei, K. Koepnik, M. Richter, *Europhysics Letters* 72 (2005) 611.
15. *A relativistic general-order multi-reference coupled cluster method: Initial implementation and application to HBr*, T. Fleig, L. K. Sørensen, J. Olsen, *Theor. Chem. Acc.* (2007), in press; published online 2 March 2007, DOI: 10.1007/s00214-007-0265-y.
16. *A Relativistic 4-Component Multi-Reference Coupled Cluster Method. Application to the CsLi Molecule*, T. Fleig, L. K. Sørensen, *NIC Symposium 2006*, **32** (2006) 91-98, Eds. G. Münster, D. Wolf, M. Kremer, NIC Series, ISBN 3-00-017351-X.
17. *Coupled-cluster response theory with linear  $r12$  corrections: The CC2-R12 model for vertical excitation energies*, H. Fliegl, C. Hättig, W. Klopper, *J. Chem. Phys.* 124 (2006) 044112.
18. *Inclusion of the (T) triples correction into the linear- $r12$  corrected coupled-cluster model CCSD(R12)*, H. Fliegl, C. Hättig, W. Klopper, *Int. J. Quant. Chem.* 106 (2006) 2306.
19. *Superconducting properties of MgB2 from first principles*, A. Floris, A. Sanna, M. Luders, G. Profeta, N. N. Lathiotakis, M. A. L. Marques, C. Franchini, E. K. U. Gross, A. Continenza, S. Massidda, *Physica C* 456 (2007) 45.
20. *Elimination of the linearization error in GW calculations based on the linearized augmented-plane-wave method*, C. Friedrich, A. Schindlmayr, S. Blügel, T. Kotani, *Phys. Rev. B* 74 (2006) 045104.
21. *Fully automated implementation of the incremental scheme: application to CCSD energies*. J. Friedrich, M. Hanrath, M. Dolg, *J. Chem. Phys.* 126 (2007) Art. No. 154110.
22. *Error analysis of incremental electron correlation calculations and application to clusters and potential energy surfaces*. J. Friedrich, M. Hanrath, M. Dolg, *Chem. Phys.* (2007) submitted, minor changes required.
23. *Energy screening for the incremental scheme. Application to intermolecular interactions*. J. Friedrich, M. Hanrath, M. Dolg, *J. Phys. Chem.* (2007) submitted, minor changes required.
24. *Molecular results for the Hartree-Fock-Wigner model*. R. Fondermann, M. Hanrath, M. Dolg, D. P. O'Neill, *Chem. Phys. Lett.* 413 (2005) 237.
25. *A quantum chemical ab initio study of the polymerization to polyhydridophosphazenes*. R. Fondermann, M. Dolg, M. Raab, E. Niecke, *Chem. Phys.* 325 (2006) 291.
26. *The performance of the Hartree-Fock-Wigner correlation model for light diatomic molecules*. R. Fondermann, M. Hanrath, M. Dolg, *Theor. Chem. Acc.* (2007) in press.
27. *Exact-exchange Methods and Perturbation Theory along the Adiabatic Connection*. A. Görling, in: *Time Dependent Functional Theory*, Editors M. Marques, C. A. Ullrich, F. Nogueira, A. Rubio, K. Burke, E. K. U. Gross (Springer, Heidelberg, 2006), p. 137.
28. *Relation between exchange-only optimized effective potential and Kohn-Sham methods with finite basis set; Solution of a paradox*. A. Görling, A. Hesselmann, M. Jones, M. Levy, *J. Chem. Phys.* (2007) submitted.

29. *A Short-Range Gradient-Corrected Density Functional in Long-Range Coupled-Cluster Calculations for Rare-Gas Dimers*, E. Goll, H.-J. Werner, H. Stoll, Phys. Chem. Chem. Phys. 7 (2005) 3917.
30. *A Short-Range Gradient-Corrected Spin Density Functional in Combination with Long-Range Coupled-Cluster Methods: Application to Alkali-Metal Rare-Gas Dimers*, E. Goll, H.-J. Werner, H. Stoll, T. Leininger, P. Gori-Giorgi, A. Savin, Chem. Phys. 329 (2006) 276.
31. *Improved Dipole Moments from Coupling Short-Range Gradient-Corrected Density Functional with Long-Range Wavefunction Based Theory*, E. Goll, H. Stoll, C. Thierfelder, P. Schwerdtfeger, Phys. Rev. A (2007) submitted.
32. *Sparse grids and related approximation schemes for higher dimensional problems*, M. Griebel, In: *Proceedings of the conference on Foundations of Computational Mathematics (FoCM05)*, Santander, Spain (2005).
33. *A wavelet based sparse grid method for the electronic Schrödinger equation*, M. Griebel, J. Hamaekers, In: *Proceedings of the International Congress of Mathematicians*, Eds. M. Sanz-Sol, J. Soria, J. Varona, J. Verdera, Vol. III, p. 1473-1506, Madrid, Spain, August 22-30, 2006. European Mathematical Society (2006).
34. *Sparse grids for the Schrödinger equation*, M. Griebel, J. Hamaekers, In: *Mathematical Modelling and Numerical Analysis*, Special volume on Computational Quantum Chemistry, Guest editor C. Le Bris (2006), in press.
35. *Discontinuity of the chemical potential in reduced-density-matrix-functional theory*, N. Helbig, N. N Lathiotakis, M. Albrecht, E. K. U. Gross, Eur. Phys. Lett. 77 (2007) 67003.
36. *Orbital Functionals in Current-Spin-Density Functional Theory*, N. Helbig, S. Kurth, S. Pittalis, E. Räsänen, E. K. U. Gross, cond-mat/0605599.
37. *Numerically stable optimized potential method with balanced Gaussian basis sets*. A. Hesselmann, A. W. Götz, F. Della Sala, A. Görling, J. Chem. Phys. (2007) in press.
38. *Failure of time-dependent density-functional methods for excitations in spatially separated systems*. W. Hieringer, A. Görling, Chem. Phys. Lett. 419 (2006) 557.
39. *3d metal nanowires and clusters inside carbon nanotubes*, V. Ivanovskaya, C. Köhler, G. Seifert, Phys. Rev. B 75 (2007) 075410.
40. *Second order Kohn-Sham perturbation theory: correlation potential for atoms in a cavity*, H. Jiang, E. Engel, J. Chem. Phys. 123 (2005) 224102.
41. *Kohn-Sham perturbation theory: Simple solution to variational instability of second order correlation energy functional*, H. Jiang, E. Engel, J. Chem. Phys. 125 (2006) 184108.
42. *Random-phase-approximation-based correlation energy functionals: Benchmark results for atoms*, H. Jiang, E. Engel, J. Chem. Phys. (2007) submitted.
43. *Local CC2 electronic excitation energies for large molecules with density-fitting*, D. Kats, T. Korona, M. Schütz, J. Chem. Phys. 125 (2006) 104106.
44. *Transition Strengths and First-Order Properties of Excited States from Local Coupled Cluster CC2 Response Theory with Density Fitting*, D. Kats, T. Korona, M. Schütz, J. Chem. Phys. (2007) in press.

45. *Relativistic formulation of the Korringa-Kohn-Rostoker coherent-potential approximation*, D. Ködderitzsch, H. Ebert, D. A. Rowlands, A. Ernst, *New Journal of Physics* 9 (2007) 81.
46. *Relativistic optimized potential method for open-shell systems*, D. Ködderitzsch, E. Engel, H. Ebert, to *Phys. Rev. B* (2007) submitted.
47. *Density functional calculations for  $Fe_n$  ( $n < 32$ )*, C. Köhler, G. Seifert, T. Frauenheim, *Chem. Phys.* 309 (2005) 23.
48. *Magnetism and the potential energy hypersurfaces of Fe53 to Fe55*, C. Köhler, G. Seifert, T. Frauenheim, *Comp. Mat. Science* 35 (2006) 297.
49. *Treatment of Collinear and Noncollinear Electron Spin within an Approximate Density Functional Based Method*, C. Köhler, T. Frauenheim, B. Hourahine, G. Seifert, M. Sternberg, *J. Phys. Chem. A*, online published (2007).
50. *Lifshitz transitions and elastic properties of Osmium under pressure*, D. Koudela, M. Richter, A. Möbius, K. Koepernik, H. Eschrig, *Phys. Rev. B* 74 (2006) 214103.
51. *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, W. Klopper, *J. Chem. Phys.* 122 (2005) 214306.
52. *Analytical nuclear gradients for the MP2-R12 method*, E. Kordel, C. Villani, W. Klopper, *Mol. Phys.*, Pulay Festschrift, submitted (2007).
53. *Time-dependent configuration-interaction calculations of laser-pulse-driven many-electron dynamics: Controlled dipole switching in lithium cyanide*, P. Krause, T. Klamroth, P. Saalfrank, *J. Chem. Phys.* 123 (2005) 074105.
54. *Dipole switching in large molecules described by explicitly Time-Dependent Configuration Interaction*, P. Krause, T. Klamroth, *J. Chem. Phys.* (2007) submitted.
55. *Molecular response properties from explicitly Time-Dependent Configuration Interaction methods*, P. Krause, T. Klamroth, P. Saalfrank, *J. Chem. Phys.* (2007) accepted.
56. *The Optimized Effective Potential Method and LDA+U*, S. Kurth, S. Pittalis, in: *Computational Nanoscience: Do It Yourself!*, J. Grotendorst, S. Blügel, D. Marx (eds.), NIC Series Vol. 31 (2006).
57. *Multipole-based integral estimates for the rigorous description of distance dependence in two-electron integrals*, D. S. Lambrecht, C. Ochsenfeld *J. Chem. Phys.* 123 (2005) 184101.
58. *Rigorous integral screening for electron correlation methods*, D. S. Lambrecht, B. Doser, C. Ochsenfeld *J. Chem. Phys.* 123 (2005) 184102.
59. *Performance of one-body reduced density-matrix functionals for the homogeneous electron gas*, N. N. Lathiotakis, N. Helbig, E. K. U. Gross, *Phys. Rev. B* 75 (2007) 195120.
60. *Direct optimization of nodal hypersurfaces in approximate wave functions*, A. Lüchow, R. Petz, T. C. Scott, *J. Chem. Phys.* 126 (2007) 144110.
61. *Explicitly correlated local second-order perturbation theory with a frozen geminal correlation factor*, F. R. Manby, H.-J. Werner, T. B. Adler, A. J. May, *J. Chem. Phys.* 124 (2006) 094103.

62. *Fast local-MP2 method with Density-Fitting for crystals. A. Theory and algorithms*, L. Maschio, D. Usvyat, F. R. Manby, S. Casassa, C. Pisani, M. Schütz, Phys. Rev. B (2007) submitted.
63. *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 72 (2005) 45125.
64. *Experimental observation and theoretical description of the pure Fano-effect in the valence-band photoemission of ferromagnets*, J. Minár, H. Ebert, C. de Nadaï, N. B. Brookes, F. Venturini, G. Ghiringhelli, L. Chioncel, A. I. Lichtenstein, M. I. Katsnelson, Phys. Rev. Lett. 95 (2005) 166401.
65. *Two-component relativistic density functional calculations of the dimers of the halogens from bromine through element 117 using effective core potential and all-electron methods*, A. V. Mitin, C. van Wüllen, J. Chem. Phys. 124 (2006) 064305.
66. *Relativistic DMRG calculations on the curve crossing of cesium hydride*, G. Moritz, M. Reiher, J. Chem. Phys. 123 (2005) 184105.
67. *Construction of environment states in quantum-chemical density matrix renormalization group calculations*, G. Moritz, M. Reiher, J. Chem. Phys. 124 (2006) 034103.
68. *Extensions of r12 corrections to CC2-R12 for excited states*, C. Neiss, C. Hättig, W. Klopper, J. Chem. Phys. 125 (2006) 064111.
69. *Frequency-dependent nonlinear optical properties with explicitly correlated coupled-cluster response theory using the CCSD(R12) model*, C. Neiss, C. Hättig, J. Chem. Phys. 126 (2007) 154101.
70. *Correlated many electron dynamics: Application to inelastic electron scattering at a metal film*, M. Nest, T. Klamroth, Phys. Rev. A 72 (2005) 012710.
71. *The Multi-Configuration Time-Dependent Hartree-Fock method for quantum chemical calculations*, M. Nest, T. Klamroth, P. Saalfrank, J. Chem. Phys. 122 (2005) 124102.
72. *Quantum carpets and correlated dynamics of several fermions*, M. Nest, Phys. Rev. A 73 (2006) 023613.
73. *Time-dependent approach to electronically excited states of molecules with the Multi-Configuration Time-Dependent Hartree-Fock method*, M. Nest, P. Ramanathan, P. Saalfrank, J. Chem. Phys. 126 (2007) 214106.
74. *Determination of the electronic ground state of molecular systems with the Multi-Configuration Time-Dependent Hartree-Fock method*, M. Nest, J. Theor. Comput. Chem. (2007) accepted.
75. *Linear-Scaling Methods in Quantum Chemistry*, C. Ochsenfeld, J. Kussmann, D. S. Lambrecht, in 'Reviews in Computational Chemistry', Vol. 23, Eds. K. B. Lipkowitz, T. R. Cundari; VCH Publishers, New York, pp. 1-82 (2007).
76. *Frozen local hole approximation*, E. Pahl, U. Birkenheuer, J. Chem. Phys. 124 (2006) 214101.
77. *The Optimized Effective Potential Method*, S. Pittalis, S. Kurth, in: *Computational Condensed Matter Physics*, S. Blügel, G. Gompper, E. Koch, H. Müller-Krumbhaar, R. Spatschek, R. G. Winkler (eds.), Schriften des Forschungszentrums Jülich, Matter and Materials Vol. 32 (2006).

78. *On the degeneracy of atomic states within exact-exchange (spin-) density functional theory*, S. Pittalis, S. Kurth, E. K. U. Gross, J. Chem. Phys. 125 (2006) 084105, and physics/0605033.
79. *Optimized Effective Potentials in Current-Spin-Density Functional Theory: an Application to Open-Shell Atoms*, S. Pittalis, S. Kurth, N. Helbig, E. K. U. Gross, Phys. Rev. A 74 (2006) 062511, and cond-mat/0609696.
80. *Recovering the degeneracy for ground states of open-shell atoms by going beyond the exact-exchange approximation*, S. Pittalis, S. Kurth, S. Sharma, E. K. U. Gross, cond-mat/0704.1593.
81. *Superconductivity in Lithium, Potassium, and Aluminum under Extreme Pressure: A First-Principles Study*, G. Profeta, C. Franchini, N. N. Lathiotakis, A. Floris, A. Sanna, M. A. L. Marques, M. Lüders, S. Massidda, E. K. U. Gross, A. Continenza, Phys. Rev. Lett. 96 (2006) 047003.
82. *Exact-Exchange Kohn-Sham formalism applied to one-dimensional periodic electronic systems*, S. Rohra, E. Engel, A. Görling, Phys. Rev. B 74 (2006) 045119.
83. *Spin-orbit interactions and spin-currents from an exact-exchange Kohn-Sham method*, S. Rohra, E. Engel, A. Görling, Phys. Rev. Lett. (2007) submitted.
84. *Laser-driven electron dynamics at interfaces*, P. Saalfrank, T. Klamroth, C. Huber, P. Krause, Isr. J. Chem. 45 (2005) 205.
85. *Superconductivity in Lithium, Potassium, and Aluminum under Extreme Pressure: A First-Principles Study*, A. Sanna, C. Franchini, A. Floris, G. Profeta, N. N. Lathiotakis, M. Lüders, M. A. L. Marques, E. K. U. Gross, A. Continenza, S. Massidda, Phys. Rev. B 73 (2006) 144512.
86. *Spin and orbital magnetism of  $Au_3Co$ : Density functional calculations*, M. Sargolzaei, I. Opahle, M. Richter, Phys. Stat. Sol. (b) 243 (2006) 286.
87. *Spin and orbital magnetism in full-Heusler alloys: A density functional theory study of  $Co_2YZ$  ( $Y = Mn, Fe$ ;  $Z = Al, Si, Ga, Ge$ )*, M. Sargolzaei, M. Richter, K. Koepf, I. Opahle, H. Eschrig, I. Chaplygin, Phys. Rev. B 74 (2006) 224410.
88. *Nodal surfaces of helium atom eigenfunctions*, T. C. Scott, A. Lüchow, D. Bressanini, J. D. Morgan, III, Phys. Rev. A 75 (2007) 060101(R).
89. *Nodal Structure of Schrödinger Wave Function: General Results and Specific Models*, T. C. Scott, A. Lüchow, J. Phys. B 40 (2007) 851.
90. *The Blue  $Xe_4^+$  Cation. Experimental Detection and Theoretical Characterization*, S. Seidel, K. Seppelt, C. van Wüllen, X. Y. Sun, Angew. Chem. (2007) accepted.
91. *Optimized Effective Potential Method for Non-Collinear Magnetism*, S. Sharma, J.K. Dewhurst, C. Ambrosch-Draxl, S. Kurth, N. Helbig, S. Pittalis, E.K.U. Gross, S. Shallcross, L. Nordström, Phys. Rev. Lett. 98 (2007) 196405, and cond-mat/0510800.
92. *Comparison of exact-exchange calculations for solids in current-spin-density- and spin-density-functional theory*, S. Sharma, S. Pittalis, S. Kurth, S. Shallcross, J.K. Dewhurst, E.K.U. Gross, cond-mat/0704.0244.

93. *Fuzzy Fragment Selection Strategies, Basis Set Dependence, and HF - DFT Comparisons in the Applications of the ADMA Method of Macromolecular Quantum Chemistry*, Z. Szekeres, T.E. Exner, P.G. Mezey, Int. J. Quantum Chem. 104 (2005) 847.
94. *Jahn-Teller distortion of the Wigner molecule in a three-electron quantum dot and a magnetic field*, M. Taut, Physica E (to appear), (Proceedings for the EP2DS Meeting 2007 in Genova)
95. *Jahn-Teller distortion of the Wigner molecule in a three-electron quantum dot and a magnetic field: pair function approach*, M. Taut, H. Eschrig, M. Richter, Phys. Rev. A (manuscript ready for submission, available on request)
96. *Quintuple- $\zeta$  quality coupled-cluster correlation energies with tripe- $\zeta$  basis sets*, D. P. Tew, W. Klopper, C. Neiss, C. Hättig, Phys. Chem. Chem. Phys. 9 (2007) 1921.
97. *Fast local-MP2 method with Density-Fitting for crystals. B. Test calculations and application to the carbon dioxide crystal*, D. Usvyat, L. Maschio, F. R. Manby, S. Casassa, M. Schütz, C. Pisani, Phys. Rev. B (2007) submitted.
98. *Embedding procedure for ab initio correlation calculations in group II metals*, E. Voloshina, N. Gaston, B. Paulus, J. Chem. Phys. 126 (2007) 134115.
99. *Wavefunction-based ab initio method for metals: application of the incremental scheme to magnesium*, E. Voloshina, B. Paulus, Phys. Rev. B (2007) in press.
100. *Correlation energies for small Mg-cluster in comparison to bulk Mg*, E. Voloshina, B. Paulus, Mol. Phys. (2007) submitted.
101. *General Orbital Invariant MP2-F12 Theory*, H.-J. Werner, T. B. Adler, F. R. Manby, J. Chem. Phys. 126 (2007) 164102.
102. *Accurate and Efficient Treatment of Two-Electron Contributions in Quasirelativistic high-order Douglas-Kroll Density Functional Calculations*, C. van Wüllen, C. Michauk, J. Chem. Phys. 123 (2005) 204113.
103. *Numerical Instabilities in the Computation of Pseudopotential Matrix Elements*, C. van Wüllen, J. Comput. Chem. 27 (2006) 135.
104. *Gradients for Two-Component Quasirelativistic Methods. Application to dihalogenides of element 116*, C. van Wüllen, N. Langermann, J. Chem. Phys. 126 (2007) 114106.
105. *Evaluation of electronic correlation contributions for optical tensors of large systems using the incremental scheme*. J. Yang, M. Dolg, J. Chem. Phys. (2007) in press.