

Publikationsliste

Hermann Stoll

2. Januar 2012

280. K.A. Peterson, C. Krause, H. Stoll, J.G. Hill, and H.-J. Werner: *Application of Explicitly Correlated Coupled-Cluster Methods to Molecules Containing Post-3d Main Group Elements*, Mol. Phys. 109 (2011) 2607
279. C. Müller, D. Usvyat and H. Stoll: *Local Correlation Methods for Solids: Comparison of Incremental and Periodic Correlation Calculations for the Argon fcc Crystal*, Phys. Rev. B 83 (2011) 245136
278. A. Stoyanova, L. Hozoi, P. Fulde and H. Stoll: *Wavefunction-Based Approach to Quasiparticle Bands: Insight into the Electronic Structure of c-ZnS*, Phys. Rev. B 83 (2011) 205119
277. R.A. Mata and H. Stoll: *An Incremental Correlation Approach to Excited State Energies Based on Natural Transition/Localized Orbitals*, J. Chem. Phys. 134 (2011) 034122
276. H. Stoll and K. Doll: *Extrapolating Wavefunction-Based Ab-Initio Results from Finite Clusters to the Bulk Solid – The Case of Group 1 and 11 Metals (Li, Cu)*, Chem. Phys. Lett. 501 (2011) 283
275. S. Chabbal, D. Jacquemin, C. Adamo, H. Stoll and Th. Leininger: *Bond Length Alternation of Conjugated Oligomers: Another Step on the Fifth Rung of Perdew’s Ladder of Functionals*, J. Chem. Phys. 133 (2010) 151104
274. B. Paulus and H. Stoll: *The Method of Increments – a Wavefunction-Based Correlation Method for Extended Systems* in: *Accurate Condensed-Phase Quantum Chemistry* (F.R. Manby, ed.), p. 57, CRC Press, Boca Raton (2010)
273. S. Chabbal, H. Stoll, H.-J. Werner and Th. Leininger: *Analytic Gradients for the Combined sr-DFT/lr-MP2 Method: Application to Weakly Bound Systems*, Mol. Phys. 108 (2010) 3373
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270. E. Goll, H.-J. Werner and H. Stoll: *Coupling of Short-Range Density-Functional with Long-Range Post-Hartree-Fock Methods*, Z. Phys. Chem. 224 (2010) 481
269. H. Stoll: *Can Incremental Expansions Cope with High-Order Coupled-Cluster Contributions?*, Mol. Phys. 108 (2010) 243

268. B. Spohn, E. Goll, H. Stoll, D. Figgen and K.A. Peterson: *Energy-Consistent Pseudopotentials for the 5d Elements — Benchmark Calculations for Oxides, Nitrides, and Pt₂*, J. Phys. Chem. A 113 (2009) 12478
267. H. Stoll, K.A. Peterson, J.M. Merritt and M.C. Heaven: *On the Ionization Potential of HfO*, J. Phys. Chem. A 113 (2009) 12353
266. A. Stoyonova, L. Hozoi, P. Fulde and H. Stoll: *Correlation-Induced Corrections to the Band Structure of Boron Nitride: A Wavefunction-Based Approach*, J. Chem. Phys. 131 (2009) 044119
265. P. Sebald, R. Oswald, P. Botschwina, H. Stoll and D. Figgen: *An Accurate Potential Energy Surface and Calculated Spectroscopic Properties for CdH₂ Isotopomers*, J. Phys. Chem. A 113 (2009) 11772
264. H. Stoll: *Towards a Wavefunction-Based Treatment of Metals — Extrapolation from Finite Clusters*, J. Phys. Chem. A 113 (2009) 11483
263. S. Santra, T. Archipov, A.B. Ene, H. Komnik, H. Stoll, E. Roduner and G. Rauhut: *Adsorption of Dioxygen to Copper in CuHY Zeolite*, Phys. Chem. Chem. Phys. 11 (2009) 8855
262. E. Goll, M. Ernst, F. Moegle-Hofacker and H. Stoll: *Development and Assessment of a Short-Range Meta-GGA Functional*, J. Chem. Phys. 130 (2009) 234112
261. R.A. Mata, H. Stoll and B.J. Costa Cabral: *A Simple One-Body Approach to the Calculation of the First Electronic Absorption Band of Water*, J. Chem. Theor. Comp. 5 (2009) 1829
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259. L. Hozoi, U. Birkenheuer, H. Stoll and P. Fulde: *Spin-State Transition and Spin-Polaron Physics in Cobalt Oxide Perovskites: Ab-Initio Approach Based on Quantum Chemical Methods*, New J. Phys. 11 (2009) 023023
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253. E. Goll, H.-J. Werner and H. Stoll: *Short-Range Density Functionals in Combination with Local Long-Range Ab-Initio Methods: Application to Non-Bonded Complexes*, Chem. Phys. 346 (2008) 257
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240. U. Birkenheuer, P. Fulde and H. Stoll: *A Simplified Method for the Computation of Correlation Effects on the Band Structure of Semiconductors*, Theor. Chem. Acc. 116 (2006) 398
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