# Christof Hattig

## List of Publications by Year in descending order

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|---|---|---|---|
| 188 papers | 17,855 citations | 22099 59 h-index | 13338 130 g-index |
| 200 all docs | 200 docs citations | 200 times ranked | 9529 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Employing Pseudopotentials to Tackle Excited-State Electron Spill-Out in Frozen Density Embedding Calculations. Journal of Chemical Theory and Computation, 2022, 18, 1737-1747. | 2.3 | 7 |
| 2 | Prediction of acid pK<sub>a</sub> values in the solvent acetone based on COSMOâ€RS. Journal of Computational Chemistry, 2022, 43, 1011-1022. | 1.5 | 4 |
| 3 | Formic Acidâ€Assisted Selective Hydrogenolysis of 5â€Hydroxymethylfurfural to 2,5â€Dimethylfuran over Bifunctional Pd Nanoparticles Supported on Nâ€Doped Mesoporous Carbon. Angewandte Chemie - International Edition, 2021, 60, 6807-6815. | 7.2 | 65 |
| 4 | AmeisensÃ‌reâ€unterstÃ¼tzte selektive Hydrogenolyse von 5â€Hydroxymethylfurfural zu 2,5â€Dimethylfuran Ã¼ber bifunktionale Pdâ€Nanopartikel auf Nâ€dotiertem mesoporÃ¶sem Kohlenstoff als TrÃ¤ger. Angewandte Chemie, 2021, 133, 6882-6891. | 1.6 | 13 |
| 5 | Tracing absorption and emission characteristics of halogen-bonded ion pairs involving halogenated imidazolium species. Physical Chemistry Chemical Physics, 2021, 23, 7480-7494. | 1.3 | 1 |
| 6 | Damped (linear) response theory within the resolution-of-identity coupled cluster singles and approximate doubles (RI-CC2) method. Journal of Chemical Physics, 2021, 154, 124110. | 1.2 | 6 |
| 7 | How Nitrogen Doping Affects Hydrogen Spillover on Carbon-Supported Pd Nanoparticles: New Insights from DFT. Journal of Physical Chemistry C, 2021, 125, 9020-9031. | 1.5 | 16 |
| 8 | Structure and Reactivity of Pristine and Reduced Spinel CoFe2O4 (001)/(100) Surfaces. Journal of Physical Chemistry C, 2021, 125, 9774-9781. | 1.5 | 8 |
| 9 | Solvent Effects in the Ultraviolet and X-ray Absorption Spectra of Pyridazine in Aqueous Solution. Journal of Physical Chemistry A, 2021, 125, 7198-7206. | 1.1 | 7 |
| 10 | An automatized workflow from molecular dynamic simulation to quantum chemical methods to identify elementary reactions and compute reaction constants. Journal of Computational Chemistry, 2021, 42, 2264-2282. | 1.5 | 6 |
| 11 | Activation of Molecular O<sub>2</sub> on CoFe<sub>2</sub>O<sub>4</sub> (001) Surfaces: An Embedded Cluster Study. Chemistry - A European Journal, 2021, 27, 17115-17126. | 1.7 | 8 |
| 12 | Magnetic Circular Dichroism of Naphthalene Derivatives: A Coupled Cluster Singles and Approximate Doubles and Time-Dependent Density Functional Theory Study. Journal of Physical Chemistry A, 2021, 125, 243-250. | 1.1 | 7 |
| 13 | Implementation of the iterative triples model CC3 for excitation energies using pair natural orbitals and Laplace transformation techniques. Journal of Chemical Physics, 2020, 153, 034109. | 1.2 | 6 |
| 14 | Magnetic circular dichroism spectra from resonant and damped coupled cluster response theory. Journal of Chemical Physics, 2020, 153, 114105. | 1.2 | 10 |
| 15 | Anchoring of palladium nanoparticles on N-doped mesoporous carbon. Physical Chemistry Chemical Physics, 2020, 22, 21317-21325. | 1.3 | 13 |
| 16 | Can Small Polyaromatics Describe Their Larger Counterparts for Local Reactions? A Computational Study on the H-Abstraction Reaction by an H-Atom from Polyaromatics. Journal of Physical Chemistry A, 2020, 124, 9626-9637. | 1.1 | 8 |
| 17 | Analytical nuclear gradients for electron-attached and electron-detached states for the second-order algebraic diagrammatic construction scheme combined with frozen-density embedding. Journal of Chemical Physics, 2020, 152, 174109. | 1.2 | 10 |
| 18 | TURBOMOLE: Modular program suite for ab initio quantum-chemical and condensed-matter simulations. Journal of Chemical Physics, 2020, 152, 184107. | 1.2 | 616 |

| # | Article | IF | Citations |
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| 19 | Comparison of Reaction Field Schemes for Coupling Continuum Solvation Models with Wave Function Methods for Excitation Energies. Journal of Chemical Theory and Computation, 2020, 16, 4554-4564. | 2.3 | 7 |
| 20 | Relaxation Dynamics of the Triazene Compound Berenil in DNA-Minor-Groove Confinement after Photoexcitation. Journal of Chemical Theory and Computation, 2020, 16, 5203-5211. | 2.3 | 1 |
| 21 | Avoiding Electron Spill-Out in QM/MM Calculations on Excited States with Simple Pseudopotentials. Journal of Chemical Theory and Computation, 2020, 16, 1373-1381. | 2.3 | 29 |
| 22 | A quantum chemical study of hydrogen adsorption on carbon-supported palladium clusters. Physical Chemistry Chemical Physics, 2019, 21, 21577-21587. | 1.3 | 13 |
| 23 | Anharmonic excited state frequencies of para-difluorobenzene, toluene and catechol using analytic RI-CC2 second derivatives. Physical Chemistry Chemical Physics, 2019, 21, 14063-14072. | 1.3 | 3 |
| 24 | UV Absorption and Magnetic Circular Dichroism Spectra of Purine, Adenine, and Guanine: A Coupled Cluster Study in Vacuo and in Aqueous Solution. Journal of Chemical Theory and Computation, 2019, 15, 1242-1254. | 2.3 | 24 |
| 25 | COSMO-RI-ADC(2) excitation energies and excited state gradients. Physical Chemistry Chemical Physics, 2018, 20, 16354-16363. | 1.3 | 33 |
| 26 | A pair natural orbital based implementation of CCSD excitation energies within the framework of linear response theory. Journal of Chemical Physics, 2018, 148, 134102. | 1.2 | 48 |
| 27 | How a linear triazene photoisomerizes in a volume-conserving fashion. Physical Chemistry Chemical Physics, 2018, 20, 28075-28087. | 1.3 | 8 |
| 28 | Analytic Excited State Gradients for the QM/MM Polarizable Embedded Second-Order Algebraic Diagrammatic Construction for the Polarization Propagator PE-ADC(2). Journal of Chemical Theory and Computation, 2018, 14, 4640-4650. | 2.3 | 13 |
| 29 | Circularly polarised fluorescence and phosphorescence calculations on organic molecules using the approximate coupled-cluster model CC2. Physical Chemistry Chemical Physics, 2018, 20, 21051-21061. | 1.3 | 5 |
| 30 | Ultrafast Dynamics of a Triazene: Excited-State Pathways and the Impact of Binding to the Minor Groove of DNA and Further Biomolecular Systems. Journal of Physical Chemistry Letters, 2017, 8, 1986-1992. | 2.1 | 11 |
| 31 | The PNOâ€“MP2 gradient and its application to molecular geometry optimisations. Molecular Physics, 2017, 115, 343-356. | 0.8 | 32 |
| 32 | Accuracy of Explicitly Correlated Local PNO-CCSD(T). Journal of Chemical Theory and Computation, 2017, 13, 2623-2633. | 2.3 | 37 |
| 33 | Combining Accuracy and Efficiency: An Incremental Focal-Point Method Based on Pair Natural Orbitals. Journal of Chemical Theory and Computation, 2017, 13, 6023-6042. | 2.3 | 14 |
| 34 | Perturbative triples correction for local pair natural orbital based explicitly correlated CCSD(F12*) using Laplace transformation techniques. Journal of Chemical Physics, 2016, 145, 234107. | 1.2 | 72 |
| 35 | Explicitly correlated second-order MÃ¸ller-Plesset perturbation theory in a Divide-Expand-Consolidate (DEC) context. Journal of Chemical Physics, 2016, 144, 204112. | 1.2 | 15 |
| 36 | Exploring the Light-Capturing Properties of Photosynthetic Chlorophyll Clusters Using Large-Scale Correlated Calculations. Journal of Chemical Theory and Computation, 2016, 12, 2644-2651. | 2.3 | 32 |

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| 37 | Spin-Free CC2 Implementation of Induced Transitions between Singlet Ground and Triplet Excited States. Journal of Chemical Theory and Computation, 2016, 12, 1892-1904. | 2.3 | 15 |
| 38 | Origin-independent two-photon circular dichroism calculations in coupled cluster theory. Physical Chemistry Chemical Physics, 2016, 18, 13683-13692. | 1.3 | 8 |
| 39 | Excited state polarizabilities for CC2 using the resolution-of-the-identity approximation. Journal of Chemical Physics, 2015, 143, 244108. | 1.2 | 10 |
| 40 | Toward assessment of density functionals for vibronic coupling in twoâ€photon absorption: A case study of 4â€nitroaniline. Journal of Computational Chemistry, 2015, 36, 1124-1131. | 1.5 | 12 |
| 41 | Polarizable Embedded RI-CC2 Method for Two-Photon Absorption Calculations. Journal of Chemical Theory and Computation, 2015, 11, 3669-3678. | 2.3 | 12 |
| 42 | Vibrational frequency scaling factors for correlation consistent basis sets and the methods CC2 and MP2 and their spin-scaled SCS and SOS variants. Journal of Chemical Physics, 2014, 141, 194106. | 1.2 | 14 |
| 43 | Turbomole. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 91-100. | 6.2 | 867 |
| 44 | The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284. | 6.2 | 1,166 |
| 45 | Bidentate cycloimidate palladium complexes with aliphatic and aromatic anagostic bonds. Chemical Communications, 2014, 50, 5909. | 2.2 | 28 |
| 46 | Optical rotation calculations on large molecules using the approximate coupled cluster model CC2 and the resolution-of-the-identity approximation. Physical Chemistry Chemical Physics, 2014, 16, 5942. | 1.3 | 14 |
| 47 | Explicitly correlated PNO-MP2 and PNO-CCSD and their application to the S66 set and large molecular systems. Physical Chemistry Chemical Physics, 2014, 16, 22167-22178. | 1.3 | 92 |
| 48 | Theoretical Study on Noncovalent Interactions in the Carbon Nanotubeâ€“Formic Acid Dimer System. Journal of Physical Chemistry C, 2014, 118, 4483-4488. | 1.5 | 8 |
| 49 | A pair natural orbital based implementation of ADC(2)-x: Perspectives and challenges for response methods for singly and doubly excited states in large molecules. Computational and Theoretical Chemistry, 2014, 1040-1041, 35-44. | 1.1 | 51 |
| 50 | Pair natural orbitals in explicitly correlated secondâ€order mÃllerâ€“plesset theory. International Journal of Quantum Chemistry, 2013, 113, 224-229. | 1.0 | 40 |
| 51 | A pair natural orbital implementation of the coupled cluster model CC2 for excitation energies. Journal of Chemical Physics, 2013, 139, 084114. | 1.2 | 104 |
| 52 | A scaling PNOâ€“MP2 method using a hybrid OSVâ€“PNO approach with an iterative direct generation of OSVs<sup>â€</sup>. Molecular Physics, 2013, 111, 2463-2476. | 0.8 | 60 |
| 53 | A combined experimental and computational study on the adsorption and reactions of NO on rutile TiO<sub>2</sub>. Physical Chemistry Chemical Physics, 2013, 15, 466-472. | 1.3 | 21 |
| 54 | Computational screening of one- and two-photon spectrally tuned channelrhodopsin mutants. Physical Chemistry Chemical Physics, 2013, 15, 7567. | 1.3 | 31 |

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| 55 | Benchmarks for 0â€“0 transitions of aromatic organic molecules: DFT/B3LYP, ADC(2), CC2, SOS-CC2 and SCS-CC2 compared to high-resolution gas-phase data. Physical Chemistry Chemical Physics, 2013, 15, 6623-6630. | 1.3 | 173 |
| 56 | Analytic Molecular Hessian Calculations for CC2 and MP2 Combined with the Resolution of Identity Approximation. Journal of Chemical Theory and Computation, 2013, 9, 1469-1480. | 2.3 | 12 |
| 57 | Large scale polarizability calculations using the approximate coupled cluster model CC2 and MP2 combined with the resolution-of-the-identity approximation. Journal of Chemical Physics, 2012, 136, 174106. | 1.2 | 27 |
| 58 | Prediction of vibrational frequencies of possible intermediates and side products of the methanol synthesis on ZnO($000overline{1}$0001Â¯) by ab initio calculations. Journal of Chemical Physics, 2012, 136, 034706. | 1.2 | 23 |
| 59 | Embedded cluster density functional and second-order MÃ¸ller-Plesset perturbation theory study on the adsorption of N2 on the rutile (110) surface. Journal of Chemical Physics, 2012, 137, 114705. | 1.2 | 6 |
| 60 | Local explicitly correlated second- and third-order MÃ¸llerâ€“Plesset perturbation theory with pair natural orbitals. Journal of Chemical Physics, 2012, 136, 204105. | 1.2 | 85 |
| 61 | Calculation of two-photon absorption strengths with the approximate coupled cluster singles and doubles model CC2 using the resolution-of-identity approximation. Physical Chemistry Chemical Physics, 2012, 14, 1175-1184. | 1.3 | 76 |
| 62 | PERIâ€“CC2: A Polarizable Embedded RI-CC2 Method. Journal of Chemical Theory and Computation, 2012, 8, 3274-3283. | 2.3 | 75 |
| 63 | Auxiliary basis sets for density-fitted correlated wavefunction calculations: weighted core-valence and ECP basis sets for post-d elements. Physical Chemistry Chemical Physics, 2012, 14, 6549. | 1.3 | 53 |
| 64 | Investigation of interstitial hydrogen and related defects in ZnO. Physical Chemistry Chemical Physics, 2012, 14, 16392. | 1.3 | 24 |
| 65 | Explicitly Correlated Electrons in Molecules. Chemical Reviews, 2012, 112, 4-74. | 23.0 | 487 |
| 66 | Quartic scaling analytical gradients of scaled opposite-spin CC2. Chemical Physics, 2012, 401, 217-227. | 0.9 | 31 |
| 67 | The chargeâ€transfer states in a stacked nucleobase dimer complex: A benchmark study. Journal of Computational Chemistry, 2011, 32, 1217-1227. | 1.5 | 73 |
| 68 | The MP2â€F12 method in the T<scp>URBOMOLE</scp> program package. Journal of Computational Chemistry, 2011, 32, 2492-2513. | 1.5 | 98 |
| 69 | Local explicitly correlated second-order MÃ¸llerâ€“Plesset perturbation theory with pair natural orbitals. Journal of Chemical Physics, 2011, 135, 074107. | 1.2 | 87 |
| 70 | Local pair natural orbitals for excited states. Journal of Chemical Physics, 2011, 135, 214106. | 1.2 | 87 |
| 71 | Scaled opposite-spin CC2 for ground and excited states with fourth order scaling computational costs. Journal of Chemical Physics, 2011, 134, 184101. | 1.2 | 91 |
| 72 | Accurate computational thermochemistry from explicitly correlated coupled-cluster theory. Theoretical Chemistry Accounts, 2010, 126, 289-304. | 0.5 | 64 |

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| 73 | Sub-meV accuracy in first-principles computations of the ionization potentials and electron affinities of the atoms H to Ne. Physical Review A, 2010, 81, . | 1.0 | 35 |
| 74 | Recent Advances in Explicitly Correlated Coupled-Cluster Response Theory for Excited States and Optical Properties. Zeitschrift Fur Physikalische Chemie, 2010, 224, 383-395. | 1.4 | 6 |
| 75 | Analytic Calculation of First-order Molecular Properties at the Explicitly-correlated Second-order MÃ¸ller-Plesset Level. Zeitschrift Fur Physikalische Chemie, 2010, 224, 695-708. | 1.4 | 11 |
| 76 | Communications: Accurate and efficient approximations to explicitly correlated coupled-cluster singles and doubles, CCSD-F12. Journal of Chemical Physics, 2010, 132, 231102. | 1.2 | 259 |
| 77 | Oxidation of 2-Propanol by Peroxo Titanium Complexes: A Combined Experimental and Theoretical Study. Journal of Physical Chemistry C, 2010, 114, 19415-19418. | 1.5 | 2 |
| 78 | Explicitly Correlated Coupled-Cluster Theory. Challenges and Advances in Computational Chemistry and Physics, 2010, , 535-572. | 0.6 | 40 |
| 79 | Analytic Calculation of First-order Molecular Properties at the Explicitly-correlated Second-order Mller-Plesset Level. , 2010, , 405-418. | | 0 |
| 80 | Highly accurate CCSD(R12) and CCSD(F12) optical response properties using standard triple-Î¶ basis sets. Journal of Chemical Physics, 2009, 131, 074102. | 1.2 | 24 |
| 81 | Structures and harmonic vibrational frequencies for excited states of diatomic molecules with CCSD(R12) and CCSD(F12) models. Journal of Chemical Physics, 2009, 130, 124101. | 1.2 | 19 |
| 82 | Formation of weakly bound, ordered adlayers of CO on rutile TiO2(110): A combined experimental and theoretical study. Journal of Chemical Physics, 2009, 130, 144703. | 1.2 | 40 |
| 83 | Automated calculation of anharmonic vibrational contributions to first hyperpolarizabilities: Quadratic response functions from vibrational configuration interaction wave functions. Journal of Chemical Physics, 2009, 131, 154101. | 1.2 | 29 |
| 84 | Preferential pathways for light-trapping involving Î²-ligated chlorophylls. Biochimica Et Biophysica Acta - Bioenergetics, 2009, 1787, 1254-1265. | 0.5 | 23 |
| 85 | Photophysics of the Trp-Gly dipeptide: Role of electron and proton transfer processes for efficient excited-state deactivation. Chemical Physics Letters, 2009, 482, 38-43. | 1.2 | 27 |
| 86 | Accurate Coupled Cluster Calculations of the Reaction Barrier Heights of Two CH<sub>3</sub><sup>â€¢</sup> + CH<sub>4</sub> Reactions. Journal of Physical Chemistry A, 2009, 113, 11679-11684. | 1.1 | 10 |
| 87 | A Density Functional Study of the Methanol Synthesis at an Oxygen Vacancy on the Polar ZnO(0001Ì…) Surface. Journal of Physical Chemistry C, 2009, 113, 1418-1425. | 1.5 | 28 |
| 88 | A diagonal orbital-invariant explicitly-correlated coupled-cluster method. Chemical Physics Letters, 2008, 452, 326-332. | 1.2 | 118 |
| 89 | Benchmarking the performance of spin-component scaled CC2 in ground and electronically excited states. Physical Chemistry Chemical Physics, 2008, 10, 4119. | 1.3 | 276 |
| 90 | Comment on Quintuple-Î¶ quality coupled-cluster correlation energies with triple-Î¶ basis sets by D. P. Tew, W. Klopper, C. Neiss and C. HÃttig, Phys. Chem. Chem. Phys., 2007, 9, 1921 [erratum]. Physical Chemistry Chemical Physics, 2008, 10, 6325. | 1.3 | 23 |

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| 91 | Frequency-dependent nonlinear optical properties with explicitly correlated coupled-cluster response theory using the CCSD(R12) model. Journal of Chemical Physics, 2007, 126, 154101. | 1.2 | 33 |
| 92 | On the internal rotations in p-cresol in its ground and first electronically excited states. Journal of Chemical Physics, 2007, 127, 024307. | 1.2 | 24 |
| 93 | Quintuple-Î¶ quality coupled-cluster correlation energies with triple-Î¶ basis sets. Physical Chemistry Chemical Physics, 2007, 9, 1921-1930. | 1.3 | 244 |
| 94 | Quantum-Chemical Investigation of the Structures and Electronic Spectra of the Nucleic Acid Bases at the Coupled Cluster CC2 Level. Journal of Physical Chemistry A, 2007, 111, 5482-5491. | 1.1 | 108 |
| 95 | Optimized accurate auxiliary basis sets for RI-MP2 and RI-CC2 calculations for the atoms Rb to Rn. Theoretical Chemistry Accounts, 2007, 117, 587-597. | 0.5 | 577 |
| 96 | Distributed memory parallel implementation of energies and gradients for second-order MÃ¸llerâ€“Plesset perturbation theory with the resolution-of-the-identity approximation. Physical Chemistry Chemical Physics, 2006, 8, 1159. | 1.3 | 223 |
| 97 | Optical Properties ofN-Succinimidyl Bithiophene and the Effects of the Binding to Biomolecules:Â Comparison between Coupled-Cluster and Time-Dependent Density Functional Theory Calculations and Experiments. Journal of Physical Chemistry B, 2006, 110, 18651-18660. | 1.2 | 26 |
| 98 | Photophysics of Organic Photostabilizers. Ab Initio Study of the Excited-State Deactivation Mechanisms of 2-(2â€˜-Hydroxyphenyl)benzotriazole. Journal of Physical Chemistry A, 2006, 110, 6301-6306. | 1.1 | 107 |
| 99 | Intramolecular Charge-Transfer Mechanism in Quinolidines:Â The Role of the Amino Twist Angle. Journal of the American Chemical Society, 2006, 128, 15672-15682. | 6.6 | 54 |
| 100 | Density dependence of electric properties of binary mixtures of inert gases. Molecular Physics, 2006, 104, 305-318. | 0.8 | 12 |
| 101 | Inclusion of the (T) triples correction into the linear-r12 corrected coupled-cluster model CCSD(R12). International Journal of Quantum Chemistry, 2006, 106, 2306-2317. | 1.0 | 69 |
| 102 | Coupled-cluster response theory with linear-r12 corrections: The CC2-R12 model for excitation energies. Journal of Chemical Physics, 2006, 124, 044112. | 1.2 | 48 |
| 103 | Benchmarking two-photon absorption with CC3 quadratic response theory, and comparison with density-functional response theory. Journal of Chemical Physics, 2006, 124, 054322. | 1.2 | 137 |
| 104 | Extensions of r12 corrections to CC2-R12 for excited states. Journal of Chemical Physics, 2006, 125, 064111. | 1.2 | 37 |
| 105 | Femtosecond pump/probe photoelectron spectroscopy of isolated C60 negative ions. Journal of Chemical Physics, 2006, 125, 074312. | 1.2 | 22 |
| 106 | Accurate Nonlinear Optical Properties for Small Molecules. Challenges and Advances in Computational Chemistry and Physics, 2006, , 51-99. | 0.6 | 23 |
| 107 | High-order correlation effects on dynamic hyperpolarizabilities and their geometric derivatives: A comparison with density functional results. Journal of Chemical Physics, 2006, 124, 114101. | 1.2 | 46 |
| 108 | Microwave and theoretical investigation of the internal rotation in m-cresol. Journal of Chemical Physics, 2006, 124, 204305. | 1.2 | 24 |

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| 109 | Coupled cluster calculations of the optical rotation of S-propylene oxide in gas phase and solution. Chemical Physics Letters, 2005, 401, 385-392. | 1.2 | 94 |
| 110 | The second hyperpolarizability of the N2 molecule calculated using the approximate coupled cluster triples model CC3. Chemical Physics Letters, 2005, 413, 272-279. | 1.2 | 11 |
| 111 | Cauchy Moments of Ne, Ar, and Kr Atoms Calculated Using the Approximate Coupled Cluster Triples Model CC3. Advances in Quantum Chemistry, 2005, , 9-21. | 0.4 | 3 |
| 112 | The accuracy ofab initiomolecular geometries for systems containing second-row atoms. Journal of Chemical Physics, 2005, 123, 184107. | 1.2 | 125 |
| 113 | Frequency-dependent hyperpolarizabilities of the Ne, Ar, and Kr atoms using the approximate coupled cluster triples model CC3. Journal of Chemical Physics, 2005, 123, 094303. | 1.2 | 12 |
| 114 | Tautomeric selectivity of the excited-state lifetime of guanine/cytosine base pairs: The role of electron-driven proton-transfer processes. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 17903-17906. | 3.3 | 290 |
| 115 | Structure Optimizations for Excited States with Correlated Second-Order Methods: CC2 and ADC(2). Advances in Quantum Chemistry, 2005, 50, 37-60. | 0.4 | 386 |
| 116 | Excited-State Intramolecular Proton Transfer:Â A Survey of TDDFT and RI-CC2 Excited-State Potential Energy Surfaces. Journal of Physical Chemistry A, 2005, 109, 3201-3208. | 1.1 | 175 |
| 117 | Optimization of auxiliary basis sets for RI-MP2 and RI-CC2 calculations: Coreâ€“valence and quintuple-Î¶ basis sets for H to Ar and QZVPP basis sets for Li to Kr. Physical Chemistry Chemical Physics, 2005, 7, 59-66. | 1.3 | 631 |
| 118 | Coupled-cluster theory with simplified linear-r12 corrections: The CCSD(R12) model. Journal of Chemical Physics, 2005, 122, 084107. | 1.2 | 167 |
| 119 | Gauge invariance of oscillator strengths in the approximate coupled cluster triples model CC3. Chemical Physics Letters, 2004, 389, 413-420. | 1.2 | 14 |
| 120 | The hyperpolarizability of the Ne atom in the approximate coupled cluster triples model CC3. Chemical Physics Letters, 2004, 391, 27-32. | 1.2 | 34 |
| 121 | The Cotton-Mouton effect of neon and argon: A benchmark study using highly correlated coupled cluster wave functions. Journal of Chemical Physics, 2004, 121, 9461-9473. | 1.2 | 16 |
| 122 | On the Nature of the Low-Lying Singlet States of 4-(Dimethyl-amino)benzonitrile. Journal of the American Chemical Society, 2004, 126, 7399-7410. | 6.6 | 113 |
| 123 | Coupled cluster calculations of the ground state potential and interaction induced electric properties of the mixed dimers of helium, neon and argon. Molecular Physics, 2004, 102, 101-110. | 0.8 | 65 |
| 124 | Ab Initio Calculation of the Vibrational and Electronic Spectra of trans- and cis-Azobenzene. Journal of the American Chemical Society, 2003, 125, 9821-9827. | 6.6 | 194 |
| 125 | OPEP: A tool for the optimal partitioning of electric properties. Journal of Computational Chemistry, 2003, 24, 997-1008. | 1.5 | 39 |
| 126 | Ab initio calculation of the refractivity and hyperpolarizability second virial coefficients of neon gas. Molecular Physics, 2003, 101, 1983-1995. | 0.8 | 30 |

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| 127 | Geometry optimizations with the coupled-cluster model CC2 using the resolution-of-the-identity approximation. Journal of Chemical Physics, 2003, 118, 7751-7761. | 1.2 | 443 |
| 128 | Analytic gradients for excited states in the coupled-cluster model CC2 employing the resolution-of-the-identity approximation. Journal of Chemical Physics, 2003, 119, 5021-5036. | 1.2 | 372 |
| 129 | Calculation of frequency-dependent polarizabilities using the approximate coupled-cluster triples model CC3. Journal of Chemical Physics, 2003, 118, 1292-1300. | 1.2 | 56 |
| 130 | A Lagrangian, integral-density direct formulation and implementation of the analytic CCSD and CCSD(T) gradients. Journal of Chemical Physics, 2003, 118, 2985-2998. | 1.2 | 57 |
| 131 | Transition moments and excited-state first-order properties in the coupled-cluster model CC2 using the resolution-of-the-identity approximation. Journal of Chemical Physics, 2002, 117, 6939-6951. | 1.2 | 402 |
| 132 | First-order properties for triplet excited states in the approximated coupled cluster model CC2 using an explicitly spin coupled basis. Journal of Chemical Physics, 2002, 116, 5401-5410. | 1.2 | 60 |
| 133 | Efficient use of the correlation consistent basis sets in resolution of the identity MP2 calculations. Journal of Chemical Physics, 2002, 116, 3175-3183. | 1.2 | 1,671 |
| 134 | The effect of intermolecular interactions on the electric properties of helium and argon. III. Quantum statistical calculations of the dielectric second virial coefficients. Journal of Chemical Physics, 2002, 117, 2609-2618. | 1.2 | 60 |
| 135 | Implementation of RI-CC2 triplet excitation energies with an application to trans-azobenzene. Physical Chemistry Chemical Physics, 2002, 4, 2111-2118. | 1.3 | 122 |
| 136 | Comment on `Efficient calculation of canonical MP2 energies' [P. Pulay, S. SaebÃ¸, K. Wolinski, Chem. Phys. Lett. 344 (2001) 543â€“552]. Chemical Physics Letters, 2002, 358, 350-353. | 1.2 | 5 |
| 137 | CC3 triplet excitation energies using an explicit spin coupled excitation space. Journal of Chemical Physics, 2001, 115, 3545-3552. | 1.2 | 24 |
| 138 | Correlated frequency-dependent electronic first hyperpolarizability of small pushâ€“pull conjugated chains. Chemical Physics Letters, 2000, 319, 327-334. | 1.2 | 75 |
| 139 | Linear response CC2 triplet excitation energies. Chemical Physics Letters, 2000, 328, 291-301. | 1.2 | 31 |
| 140 | Triplet excitation energies in the coupled cluster singles and doubles model using an explicit triplet spin coupled excitation space. Journal of Chemical Physics, 2000, 113, 7765-7772. | 1.2 | 40 |
| 141 | Gauge-origin independent magneto-optical activity within coupled cluster response theory. Journal of Chemical Physics, 2000, 113, 3561-3572. | 1.2 | 64 |
| 142 | Distributed first and second order hyperpolarizabilities: An improved calculation of nonlinear optical susceptibilities of molecular crystals. Journal of Chemical Physics, 2000, 112, 6161-6172. | 1.2 | 55 |
| 143 | Ab initio study of the electric-field-gradient-induced birefringence of a polar molecule: CO. Journal of Chemical Physics, 2000, 113, 3077-3087. | 1.2 | 36 |
| 144 | CC2 excitation energy calculations on large molecules using the resolution of the identity approximation. Journal of Chemical Physics, 2000, 113, 5154. | 1.2 | 1,319 |

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| 145 | Dispersion coefficients for second hyperpolarizabilities using coupled cluster cubic response theory. Advances in Quantum Chemistry, 1999, , 111-148. | 0.4 | 15 |
| 146 | The effect of intermolecular interactions on the electric properties of helium and argon. I. Ab initio calculation of the interaction induced polarizability and hyperpolarizability in He2 and Ar2. Journal of Chemical Physics, 1999, 111, 10099-10107. | 1.2 | 75 |
| 147 | Gauge invariant coupled cluster response theory. Journal of Chemical Physics, 1999, 110, 8318-8327. | 1.2 | 96 |
| 148 | The effect of intermolecular interactions on the electric properties of helium and argon. II. The dielectric, refractivity, Kerr, and hyperpolarizability second virial coefficients. Journal of Chemical Physics, 1999, 111, 10108-10118. | 1.2 | 48 |
| 149 | Ab initiocalculation of the frequency-dependent interaction induced hyperpolarizability of Ar2. Journal of Chemical Physics, 1999, 110, 2872-2882. | 1.2 | 46 |
| 150 | The electric-field-gradient-induced birefringence of Helium, Neon, Argon, and SF6. Journal of Chemical Physics, 1999, 111, 7828-7836. | 1.2 | 26 |
| 151 | Ground and excited state polarizabilities and dipole transition properties of benzene from coupled cluster response theory. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1999, 55, 509-524. | 2.0 | 37 |
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