# Christof Hattig

## List of Publications by Citations

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|---|---|---|---|
| 188 papers | 15,318 citations | 56 h-index | 121 g-index |
| 198 ext. papers | 16,590 ext. citations | 4.1 avg, IF | 6.87 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 188 | Efficient use of the correlation consistent basis sets in resolution of the identity MP2 calculations. *Journal of Chemical Physics*, **2002**, 116, 3175-3183 | 3.9 | 1456 |
| 187 | CC2 excitation energy calculations on large molecules using the resolution of the identity approximation. *Journal of Chemical Physics*, **2000**, 113, 5154 | 3.9 | 1207 |
| 186 | The Dalton quantum chemistry program system. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 269-284 | 7.9 | 956 |
| 185 | Turbomole. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 91-100 | 7.9 | 710 |
| 184 | Optimization of auxiliary basis sets for RI-MP2 and RI-CC2 calculations: Core□valence and quintuple-□basis sets for H to Ar and QZVPP basis sets for Li to Kr. *Physical Chemistry Chemical Physics*, **2005**, 7, 59-66 | 3.6 | 552 |
| 183 | Response functions from Fourier component variational perturbation theory applied to a time-averaged quasienergy. *International Journal of Quantum Chemistry*, **1998**, 68, 1-52 | 2.1 | 454 |
| 182 | Explicitly correlated electrons in molecules. *Chemical Reviews*, **2012**, 112, 4-74 | 68.1 | 419 |
| 181 | Geometry optimizations with the coupled-cluster model CC2 using the resolution-of-the-identity approximation. *Journal of Chemical Physics*, **2003**, 118, 7751-7761 | 3.9 | 412 |
| 180 | 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 | 1.9 | 396 |
| 179 | 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 | 3.9 | 375 |
| 178 | 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 | 3.9 | 341 |
| 177 | Structure Optimizations for Excited States with Correlated Second-Order Methods: CC2 and ADC(2). *Advances in Quantum Chemistry*, **2005**, 50, 37-60 | 1.4 | 320 |
| 176 | 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, 17903-6 | 11.5 | 270 |
| 175 | TURBOMOLE: Modular program suite for ab initio quantum-chemical and condensed-matter simulations. *Journal of Chemical Physics*, **2020**, 152, 184107 | 3.9 | 255 |
| 174 | Benchmarking the performance of spin-component scaled CC2 in ground and electronically excited states. *Physical Chemistry Chemical Physics*, **2008**, 10, 4119-27 | 3.6 | 233 |
| 173 | Communications: Accurate and efficient approximations to explicitly correlated coupled-cluster singles and doubles, CCSD-F12. *Journal of Chemical Physics*, **2010**, 132, 231102 | 3.9 | 226 |
| 172 | Quintuple-zeta quality coupled-cluster correlation energies with triple-zeta basis sets. *Physical Chemistry Chemical Physics*, **2007**, 9, 1921-30 | 3.6 | 223 |

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| 171 | Distributed memory parallel implementation of energies and gradients for second-order Møller-Plesset perturbation theory with the resolution-of-the-identity approximation. *Physical Chemistry Chemical Physics*, **2006**, 8, 1159-69 | 3.6 | 192 |
| 170 | Ab initio calculation of the vibrational and electronic spectra of trans- and cis-azobenzene. *Journal of the American Chemical Society*, **2003**, 125, 9821-7 | 16.4 | 168 |
| 169 | Excited-state intramolecular proton transfer: a survey of TDDFT and RI-CC2 excited-state potential energy surfaces. *Journal of Physical Chemistry A*, **2005**, 109, 3201-8 | 2.8 | 165 |
| 168 | Coupled-cluster theory with simplified linear-r(12) corrections: the CCSD(R12) model. *Journal of Chemical Physics*, **2005**, 122, 84107 | 3.9 | 158 |
| 167 | Benchmarks for 0-0 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, 6623-30 | 3.6 | 153 |
| 166 | Distributed polarizabilities using the topological theory of atoms in molecules. *Chemical Physics Letters*, **1994**, 219, 267-273 | 2.5 | 136 |
| 165 | Benchmarking two-photon absorption with CC3 quadratic response theory, and comparison with density-functional response theory. *Journal of Chemical Physics*, **2006**, 124, 054322 | 3.9 | 125 |
| 164 | Polarizabilities of CO, N2, HF, Ne, BH, and CH+ from ab initio calculations: Systematic studies of electron correlation, basis set errors, and vibrational contributions. *Journal of Chemical Physics*, **1998**, 109, 4745-4757 | 3.9 | 120 |
| 163 | Frequency-dependent first hyperpolarizabilities using coupled cluster quadratic response theory. *Chemical Physics Letters*, **1997**, 269, 428-434 | 2.5 | 119 |
| 162 | Implementation of RI-CC2 triplet excitation energies with an application to trans-azobenzene. *Physical Chemistry Chemical Physics*, **2002**, 4, 2111-2118 | 3.6 | 114 |
| 161 | A diagonal orbital-invariant explicitly-correlated coupled-cluster method. *Chemical Physics Letters*, **2008**, 452, 326-332 | 2.5 | 113 |
| 160 | The accuracy of ab initio molecular geometries for systems containing second-row atoms. *Journal of Chemical Physics*, **2005**, 123, 184107 | 3.9 | 113 |
| 159 | On the nature of the low-lying singlet states of 4-(Dimethyl-amino)benzonitrile. *Journal of the American Chemical Society*, **2004**, 126, 7399-410 | 16.4 | 108 |
| 158 | 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, 5482-91 | 2.8 | 106 |
| 157 | Photophysics of organic photostabilizers. Ab initio study of the excited-state deactivation mechanisms of 2-(2'-hydroxyphenyl)benzotriazole. *Journal of Physical Chemistry A*, **2006**, 110, 6301-6 | 2.8 | 104 |
| 156 | Frequency-dependent second hyperpolarizabilities using coupled cluster cubic response theory. *Chemical Physics Letters*, **1998**, 282, 139-146 | 2.5 | 101 |
| 155 | The MP2-F12 method in the Turbomole program package. *Journal of Computational Chemistry*, **2011**, 32, 2492-513 | 3.5 | 92 |
| 154 | Coupled cluster calculations of the optical rotation of S-propylene oxide in gas phase and solution. *Chemical Physics Letters*, **2005**, 401, 385-392 | 2.5 | 92 |

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| 153 | Gauge invariant coupled cluster response theory. *Journal of Chemical Physics*, **1999**, 110, 8318-8327 | 3.9 | 87 |
| 152 | A pair natural orbital implementation of the coupled cluster model CC2 for excitation energies. *Journal of Chemical Physics*, **2013**, 139, 084114 | 3.9 | 82 |
| 151 | Explicitly correlated PNO-MP2 and PNO-CCSD and their application to the S66 set and large molecular systems. *Physical Chemistry Chemical Physics*, **2014**, 16, 22167-78 | 3.6 | 80 |
| 150 | Polarizabilities and first hyperpolarizabilities of HF, Ne, and BH from full configuration interaction and coupled cluster calculations. *Journal of Chemical Physics*, **1999**, 111, 1917-1925 | 3.9 | 80 |
| 149 | Local explicitly correlated second- and third-order Møller-Plesset perturbation theory with pair natural orbitals. *Journal of Chemical Physics*, **2012**, 136, 204105 | 3.9 | 79 |
| 148 | Multiphoton transition moments and absorption cross sections in coupled cluster response theory employing variational transition moment functionals. *Journal of Chemical Physics*, **1998**, 108, 8331-8354 | 3.9 | 77 |
| 147 | Local explicitly correlated second-order Møller-Plesset perturbation theory with pair natural orbitals. *Journal of Chemical Physics*, **2011**, 135, 074107 | 3.9 | 75 |
| 146 | Scaled opposite-spin CC2 for ground and excited states with fourth order scaling computational costs. *Journal of Chemical Physics*, **2011**, 134, 184101 | 3.9 | 74 |
| 145 | Correlated frequency-dependent electronic first hyperpolarizability of small push–pull conjugated chains. *Chemical Physics Letters*, **2000**, 319, 327-334 | 2.5 | 74 |
| 144 | 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 | 3.9 | 74 |
| 143 | Local pair natural orbitals for excited states. *Journal of Chemical Physics*, **2011**, 135, 214106 | 3.9 | 73 |
| 142 | The charge-transfer states in a stacked nucleobase dimer complex: a benchmark study. *Journal of Computational Chemistry*, **2011**, 32, 1217-27 | 3.5 | 67 |
| 141 | PERI-CC2: A Polarizable Embedded RI-CC2 Method. *Journal of Chemical Theory and Computation*, **2012**, 8, 3274-83 | 6.4 | 66 |
| 140 | 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 | 2.1 | 66 |
| 139 | Perturbative triples correction for local pair natural orbital based explicitly correlated CCSD(F12*) using Laplace transformation techniques. *Journal of Chemical Physics*, **2016**, 145, 234107 | 3.9 | 63 |
| 138 | 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 | 1.7 | 60 |
| 137 | Ab initio study of the individual interaction energy components in the ground state of the mercury dimer. *Molecular Physics*, **1996**, 89, 139-156 | 1.7 | 60 |
| 136 | TDMP2 calculation of dynamic multipole polarizabilities and dispersion coefficients for the halogen anions F⁻, Cl⁻, Br⁻ and I⁻. *Journal of Chemical Physics*, **1998**, 108, 3863-3870 | 3.9 | 58 |

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| 135 | Correlated frequency-dependent polarizabilities and dispersion coefficients in the time-dependent second-order M□ller-Plesset approximation. *Chemical Physics Letters*, **1995**, 233, 359-370 | 2.5 | 58 |
| 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 | 3.9 | 57 |
| 133 | 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, 1175-84 | 3.6 | 56 |
| 132 | TDMP2 Calculation of Dynamic Multipole Polarizabilities and Dispersion Coefficients of the Noble Gases Ar, Kr, Xe, and Rn. *The Journal of Physical Chemistry*, **1996**, 100, 6243-6248 | | 56 |
| 131 | A scaling PNO□MP2 method using a hybrid OSV□PNO approach with an iterative direct generation of OSVs□*Molecular Physics*, **2013**, 111, 2463-2476 | 1.7 | 55 |
| 130 | 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 | 3.9 | 55 |
| 129 | Gauge-origin independent magneto-optical activity within coupled cluster response theory. *Journal of Chemical Physics*, **2000**, 113, 3561-3572 | 3.9 | 55 |
| 128 | Accurate computational thermochemistry from explicitly correlated coupled-cluster theory. *Theoretical Chemistry Accounts*, **2010**, 126, 289-304 | 1.9 | 54 |
| 127 | A Lagrangian, integral-density direct formulation and implementation of the analytic CCSD and CCSD(T) gradients. *Journal of Chemical Physics*, **2003**, 118, 2985-2998 | 3.9 | 54 |
| 126 | Intramolecular charge-transfer mechanism in quinolidines: the role of the amino twist angle. *Journal of the American Chemical Society*, **2006**, 128, 15672-82 | 16.4 | 51 |
| 125 | Calculation of frequency-dependent polarizabilities using the approximate coupled-cluster triples model CC3. *Journal of Chemical Physics*, **2003**, 118, 1292-1300 | 3.9 | 51 |
| 124 | Distributed first and second order hyperpolarizabilities: An improved calculation of nonlinear optical susceptibilities of molecular crystals. *Journal of Chemical Physics*, **2000**, 112, 6161-6172 | 3.9 | 51 |
| 123 | Cauchy moments and dispersion coefficients using coupled cluster linear response theory. *Journal of Chemical Physics*, **1997**, 107, 10592-10598 | 3.9 | 49 |
| 122 | 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 | 2 | 46 |
| 121 | Coupled-cluster response theory with linear-r12 corrections: the CC2-R12 model for excitation energies. *Journal of Chemical Physics*, **2006**, 124, 044112 | 3.9 | 46 |
| 120 | Ab initio calculation of the frequency-dependent interaction induced hyperpolarizability of Ar2. *Journal of Chemical Physics*, **1999**, 110, 2872-2882 | 3.9 | 46 |
| 119 | High-order correlation effects on dynamic hyperpolarizabilities and their geometric derivatives: a comparison with density functional results. *Journal of Chemical Physics*, **2006**, 124, 114101 | 3.9 | 45 |
| 118 | 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 | 3.9 | 44 |

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| 117 | Intermolecular interaction energies by topologically partitioned electric properties II. Dispersion energies in one-centre and multicentre multipole expansions. *Molecular Physics*, **1997**, 91, 145-160 | 1.7 | 43 |
| 116 | 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, 6549-55 | 3.6 | 42 |
| 115 | Coupled cluster calculations of the frequency-dependent second hyperpolarizabilities of Ne, Ar, N2, and CH4. *Journal of Chemical Physics*, **1998**, 109, 2762-2778 | 3.9 | 40 |
| 114 | Explicitly Correlated Coupled-Cluster Theory. *Challenges and Advances in Computational Chemistry and Physics*, **2010**, 535-572 | 0.7 | 39 |
| 113 | Pair natural orbitals in explicitly correlated second-order m□ller□plesset theory. *International Journal of Quantum Chemistry*, **2013**, 113, 224-229 | 2.1 | 38 |
| 112 | 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 | 3.9 | 38 |
| 111 | Coupled cluster investigation of the electric-field-gradient-induced birefringence of H2, N2, C2H2, and CH4. *Journal of Chemical Physics*, **1998**, 109, 7176-7184 | 3.9 | 38 |
| 110 | Coupled cluster response calculations of two-photon transition probability rate constants for helium, neon and argon. *Journal of Chemical Physics*, **1998**, 108, 8355-8359 | 3.9 | 38 |
| 109 | OPEP: a tool for the optimal partitioning of electric properties. *Journal of Computational Chemistry*, **2003**, 24, 997-1008 | 3.5 | 37 |
| 108 | Static and frequency-dependent polarizabilities of excited singlet states using coupled cluster response theory. *Journal of Chemical Physics*, **1998**, 109, 9237-9243 | 3.9 | 36 |
| 107 | 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 | 4.4 | 36 |
| 106 | Recurrence relations for the direct calculation of spherical multipole interaction tensors and Coulomb-type interaction energies. *Chemical Physics Letters*, **1996**, 260, 341-351 | 2.5 | 36 |
| 105 | Extensions of r12 corrections to CC2-R12 for excited states. *Journal of Chemical Physics*, **2006**, 125, 64113 | 3.9 | 34 |
| 104 | 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 | 3.9 | 34 |
| 103 | Ab initio study of the electric-field-gradient-induced birefringence of a polar molecule: CO. *Journal of Chemical Physics*, **2000**, 113, 3077-3087 | 3.9 | 33 |
| 102 | A pair natural orbital based implementation of CCSD excitation energies within the framework of linear response theory. *Journal of Chemical Physics*, **2018**, 148, 134102 | 3.9 | 32 |
| 101 | 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, | 2.6 | 32 |
| 100 | The hyperpolarizability of the Ne atom in the approximate coupled cluster triples model CC3. *Chemical Physics Letters*, **2004**, 391, 27-32 | 2.5 | 32 |

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| 99 | Intermolecular interaction energies by topologically partitioned electric properties. 1. Electrostatic and induction energies in one-centre and multicentre multipole expansions. *Molecular Physics*, **1996**, 88, 69-92 | 1.7 | 32 |
| 98 | Accuracy of Explicitly Correlated Local PNO-CCSD(T). *Journal of Chemical Theory and Computation*, **2017**, 13, 2623-2633 | 6.4 | 31 |
| 97 | Frequency-dependent nonlinear optical properties with explicitly correlated coupled-cluster response theory using the CCSD(R12) model. *Journal of Chemical Physics*, **2007**, 126, 154101 | 3.9 | 31 |
| 96 | Ab initio calculation of the refractivity and hyperpolarizability second virial coefficients of neon gas. *Molecular Physics*, **2003**, 101, 1983-1995 | 1.7 | 29 |
| 95 | 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 | 3.9 | 28 |
| 94 | The PNO-MP2 gradient and its application to molecular geometry optimisations. *Molecular Physics*, **2017**, 115, 343-356 | 1.7 | 27 |
| 93 | Linear response CC2 triplet excitation energies. *Chemical Physics Letters*, **2000**, 328, 291-301 | 2.5 | 27 |
| 92 | TDMP2 calculation of dynamic multipole polarizabilities and dispersion coefficients of the triplebonded molecules CO, N2, CN□and NO+. *Journal of Chemical Physics*, **1996**, 105, 9948-9965 | 3.9 | 27 |
| 91 | Transferability of topologically partitioned polarizabilities: the case of n-alkanes. *Molecular Physics*, **1996**, 89, 595-605 | 1.7 | 27 |
| 90 | Bidentate cycloimidate palladium complexes with aliphatic and aromatic anagostic bonds. *Chemical Communications*, **2014**, 50, 5909-11 | 5.8 | 26 |
| 89 | 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 | 2.5 | 26 |
| 88 | Derivation of coupled cluster excited states response functions and multiphoton transition moments between two excited states as derivatives of variational functionals. *Journal of Chemical Physics*, **1998**, 109, 9219-9236 | 3.9 | 26 |
| 87 | Exploring the Light-Capturing Properties of Photosynthetic Chlorophyll Clusters Using Large-Scale Correlated Calculations. *Journal of Chemical Theory and Computation*, **2016**, 12, 2644-51 | 6.4 | 26 |
| 86 | Computational screening of one- and two-photon spectrally tuned channelrhodopsin mutants. *Physical Chemistry Chemical Physics*, **2013**, 15, 7567-76 | 3.6 | 25 |
| 85 | Quartic scaling analytical gradients of scaled opposite-spin CC2. *Chemical Physics*, **2012**, 401, 217-227 | 2.3 | 25 |
| 84 | The electric-field-gradient-induced birefringence of Helium, Neon, Argon, and SF6. *Journal of Chemical Physics*, **1999**, 111, 7828-7836 | 3.9 | 25 |
| 83 | Dispersion formulas for hyperpolarizability averages. *Molecular Physics*, **1998**, 94, 455-460 | 1.7 | 25 |
| 82 | Highly accurate CCSD(R12) and CCSD(F12) optical response properties using standard triple-zeta basis sets. *Journal of Chemical Physics*, **2009**, 131, 074102 | 3.9 | 24 |

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| 81 | 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 | 3.0 | 24 |
| 80 | Calculation of orientation-dependent double-tensor moments for Coulomb-type intermolecular interactions. *Molecular Physics*, **1994**, 81, 813-824 | 1.7 | 24 |
| 79 | Preferential pathways for light-trapping involving beta-ligated chlorophylls. *Biochimica Et Biophysica Acta - Bioenergetics*, **2009**, 1787, 1254-65 | 4.6 | 23 |
| 78 | Prediction of vibrational frequencies of possible intermediates and side products of the methanol synthesis on ZnO(0001) by ab initio calculations. *Journal of Chemical Physics*, **2012**, 136, 034706 | 3.9 | 23 |
| 77 | A basis set study of coupled cluster and full configuration interaction calculations of molecular electric properties for BH. *Chemical Physics Letters*, **1998**, 291, 536-546 | 2.5 | 23 |
| 76 | Optical properties of N-succinimidyl bithiophene and the effects of the binding to biomolecules: comparison between coupled-cluster and time-dependent density functional theory calculations and experiments. *Journal of Physical Chemistry B*, **2006**, 110, 18651-60 | 3.4 | 23 |
| 75 | CC3 triplet excitation energies using an explicit spin coupled excitation space. *Journal of Chemical Physics*, **2001**, 115, 3545-3552 | 3.9 | 23 |
| 74 | Topologically partitioned dynamic polarizabilities using the theory of atoms in molecules. *Canadian Journal of Chemistry*, **1996**, 74, 976-987 | 0.9 | 23 |
| 73 | A Density Functional Study of the Methanol Synthesis at an Oxygen Vacancy on the Polar ZnO(0001 ) Surface. *Journal of Physical Chemistry C*, **2009**, 113, 1418-1425 | 3.8 | 22 |
| 72 | Dispersion coefficients for first hyperpolarizabilities using coupled cluster quadratic response theory. *Theoretical Chemistry Accounts*, **1998**, 100, 230-240 | 1.9 | 22 |
| 71 | COSMO-RI-ADC(2) excitation energies and excited state gradients. *Physical Chemistry Chemical Physics*, **2018**, 20, 16354-16363 | 3.6 | 21 |
| 70 | A combined experimental and computational study on the adsorption and reactions of NO on rutile TiO2. *Physical Chemistry Chemical Physics*, **2013**, 15, 466-72 | 3.6 | 21 |
| 69 | Comment on Quintuple-ζ quality coupled-cluster correlation energies with triple-ζ basis sets by D. P. Tew, W. Klopper, C. Neiss and C. Hättig, Phys. Chem. Chem. Phys., 2007, 9, 1921 [erratum]. *Physical Chemistry Chemical Physics*, **2008**, 10, 6325 | 3.6 | 21 |
| 68 | Response functions from Fourier component variational perturbation theory applied to a time-averaged quasienergy **1998**, 68, 1 | | 21 |
| 67 | Investigation of interstitial hydrogen and related defects in ZnO. *Physical Chemistry Chemical Physics*, **2012**, 14, 16392-9 | 3.6 | 20 |
| 66 | Femtosecond pump/probe photoelectron spectroscopy of isolated C60 negative ions. *Journal of Chemical Physics*, **2006**, 125, 074312 | 3.9 | 20 |
| 65 | Accurate Nonlinear Optical Properties for Small Molecules. *Challenges and Advances in Computational Chemistry and Physics*, **2006**, 51-99 | 0.7 | 20 |
| 64 | Coupled cluster calculations of Verdet constants. *Chemical Physics Letters*, **1997**, 281, 445-451 | 2.5 | 19 |

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| 63 | On the internal rotations in p-cresol in its ground and first electronically excited states. *Journal of Chemical Physics*, **2007**, 127, 024307 | 3.9 | 19 |
| 62 | 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 | 3.9 | 18 |
| 61 | Microwave and theoretical investigation of the internal rotation in m-cresol. *Journal of Chemical Physics*, **2006**, 124, 204305 | 3.9 | 18 |
| 60 | Avoiding Electron Spill-Out in QM/MM Calculations on Excited States with Simple Pseudopotentials. *Journal of Chemical Theory and Computation*, **2020**, 16, 1373-1381 | 6.4 | 16 |
| 59 | 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 | 6.4 | 16 |
| 58 | Formic Acid-Assisted Selective Hydrogenolysis of 5-Hydroxymethylfurfural to 2,5-Dimethylfuran over Bifunctional Pd Nanoparticles Supported on N-Doped Mesoporous Carbon. *Angewandte Chemie - International Edition*, **2021**, 60, 6807-6815 | 16.4 | 16 |
| 57 | The Cotton-Mouton effect of neon and argon: a benchmark study using highly correlated coupled cluster wave functions. *Journal of Chemical Physics*, **2004**, 121, 9461-73 | 3.9 | 15 |
| 56 | Dispersion coefficients for second hyperpolarizabilities using coupled cluster cubic response theory. *Advances in Quantum Chemistry*, **1999**, 111-148 | 1.4 | 13 |
| 55 | Toward assessment of density functionals for vibronic coupling in two-photon absorption: A case study of 4-nitroaniline. *Journal of Computational Chemistry*, **2015**, 36, 1124-31 | 3.5 | 12 |
| 54 | 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 | 3.9 | 12 |
| 53 | Analytic Molecular Hessian Calculations for CC2 and MP2 Combined with the Resolution of Identity Approximation. *Journal of Chemical Theory and Computation*, **2013**, 9, 1469-80 | 6.4 | 12 |
| 52 | Density dependence of electric properties of binary mixtures of inert gases. *Molecular Physics*, **2006**, 104, 305-318 | 1.7 | 12 |
| 51 | Gauge invariance of oscillator strengths in the approximate coupled cluster triples model CC3. *Chemical Physics Letters*, **2004**, 389, 413-420 | 2.5 | 12 |
| 50 | Polarizable Embedded RI-CC2 Method for Two-Photon Absorption Calculations. *Journal of Chemical Theory and Computation*, **2015**, 11, 3669-78 | 6.4 | 11 |
| 49 | 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, 5942-51 | 3.6 | 11 |
| 48 | Analytic Calculation of First-order Molecular Properties at the Explicitly-correlated Second-order M□ller-Plesset Level. *Zeitschrift Fur Physikalische Chemie*, **2010**, 224, 695-708 | 3.1 | 11 |
| 47 | Frequency-dependent hyperpolarizabilities of the Ne, Ar, and Kr atoms using the approximate coupled cluster triples model CC3. *Journal of Chemical Physics*, **2005**, 123, 94303 | 3.9 | 11 |
| 46 | Comment on □requency-dependent equation-of-motion coupled cluster hyperpolarizabilities: Resolution of the discrepancy between theory and experiment for HF?□J. Chem. Phys. 107, 10823 (1997)]. *Journal of Chemical Physics*, **1998**, 109, 3293-3295 | 3.9 | 11 |

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| 45 | Response functions from Fourier component variational perturbation theory applied to a time-averaged quasienergy **1998**, 68, 1 | | 11 |
| 44 | Combining Accuracy and Efficiency: An Incremental Focal-Point Method Based on Pair Natural Orbitals. *Journal of Chemical Theory and Computation*, **2017**, 13, 6023-6042 | 6.4 | 10 |
| 43 | Excited state polarizabilities for CC2 using the resolution-of-the-identity approximation. *Journal of Chemical Physics*, **2015**, 143, 244108 | 3.9 | 10 |
| 42 | The second hyperpolarizability of the N2 molecule calculated using the approximate coupled cluster triples model CC3. *Chemical Physics Letters*, **2005**, 413, 272-279 | 2.5 | 10 |
| 41 | Explicitly correlated second-order Møller-Plesset perturbation theory in a Divide-Expand-Consolidate (DEC) context. *Journal of Chemical Physics*, **2016**, 144, 204112 | 3.9 | 10 |
| 40 | 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 | 6.4 | 9 |
| 39 | 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 | 6.4 | 9 |
| 38 | Accurate coupled cluster calculations of the reaction barrier heights of two CH3* + CH4 reactions. *Journal of Physical Chemistry A*, **2009**, 113, 11679-84 | 2.8 | 9 |
| 37 | On the calculation of derivatives for Coulomb-type interaction energies and general anisotropic pair potentials. *Chemical Physics Letters*, **1997**, 268, 521-530 | 2.5 | 9 |
| 36 | Spin-Free CC2 Implementation of Induced Transitions between Singlet Ground and Triplet Excited States. *Journal of Chemical Theory and Computation*, **2016**, 12, 1892-904 | 6.4 | 9 |
| 35 | Dispersion coefficients for polarizabilities and first and second hyperpolarizabilities using full configuration interaction theory. *Chemical Physics Letters*, **1999**, 307, 235-243 | 2.5 | 8 |
| 34 | Theoretical Study on Noncovalent Interactions in the Carbon Nanotube–Formic Acid Dimer System. *Journal of Physical Chemistry C*, **2014**, 118, 4483-4488 | 3.8 | 7 |
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