# Hans Lischka

List of Publications by Year
in descending order

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|---|---|---|---|
| 315 papers | 16,575 citations | 14614 66 h-index | 20900 115 g-index |
| 323 all docs | 323 docs citations | 323 times ranked | 10247 citing authors |

| # | Article | IF | Citations |
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| 1 | <scp>Molcas</scp> 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. Journal of Computational Chemistry, 2016, 37, 506-541. | 1.5 | 1,317 |
| 2 | Multiconfiguration Self-Consistent Field and Multireference Configuration Interaction Methods and Applications. Chemical Reviews, 2012, 112, 108-181. | 23.0 | 559 |
| 3 | The on-the-fly surface-hopping program system Newton-X: Application to ab initio simulation of the nonadiabatic photodynamics of benchmark systems. Journal of Photochemistry and Photobiology A: Chemistry, 2007, 190, 228-240. | 2.0 | 422 |
| 4 | High-level multireference methods in the quantum-chemistry program system COLUMBUS: Analytic MR-CISD and MR-AQCC gradients and MR-AQCC-LRT for excited states, GUGA spinâ€“orbit CI and parallel CI density. Physical Chemistry Chemical Physics, 2001, 3, 664-673. | 1.3 | 401 |
| 5 | Analysis of Excitonic and Charge Transfer Interactions from Quantum Chemical Calculations. Journal of Chemical Theory and Computation, 2012, 8, 2777-2789. | 2.3 | 375 |
| 6 | Newtonâ€<scp>X</scp>: a surfaceâ€hopping program for nonadiabatic molecular dynamics. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 26-33. | 6.2 | 370 |
| 7 | Relaxation mechanisms of UV-photoexcited DNA and RNA nucleobases. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 21453-21458. | 3.3 | 362 |
| 8 | A progress report on the status of the COLUMBUSMRCI program system. International Journal of Quantum Chemistry, 1988, 34, 149-165. | 1.0 | 353 |
| 9 | Analytic evaluation of nonadiabatic coupling terms at the MR-CI level. I. Formalism. Journal of Chemical Physics, 2004, 120, 7322-7329. | 1.2 | 290 |
| 10 | Multireference Approaches for Excited States of Molecules. Chemical Reviews, 2018, 118, 7293-7361. | 23.0 | 287 |
| 11 | Analytic evaluation of nonadiabatic coupling terms at the MR-CI level. II. Minima on the crossing seam: Formaldehyde and the photodimerization of ethylene. Journal of Chemical Physics, 2004, 120, 7330-7339. | 1.2 | 216 |
| 12 | The UV absorption of nucleobases: semi-classical ab initio spectra simulations. Physical Chemistry Chemical Physics, 2010, 12, 4959. | 1.3 | 208 |
| 13 | The Multiradical Character of Oneâ€•and Twoâ€Dimensional Graphene Nanoribbons. Angewandte Chemie - International Edition, 2013, 52, 2581-2584. | 7.2 | 197 |
| 14 | Nonadiabatic Deactivation of 9H-Adenine: A Comprehensive Picture Based on Mixed Quantumâ^'Classical Dynamics. Journal of the American Chemical Society, 2008, 130, 6831-6839. | 6.6 | 191 |
| 15 | Wettability of kaolinite (001) surfaces â€" Molecular dynamic study. Geoderma, 2011, 169, 47-54. | 2.3 | 176 |
| 16 | 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 |
| 17 | Ultrafast internal conversion pathway and mechanism in 2-(2â€²-hydroxyphenyl)benzothiazole: a case study for excited-state intramolecular proton transfer systems. Physical Chemistry Chemical Physics, 2009, 11, 1406. | 1.3 | 174 |
| 18 | Surface hopping dynamics using a locally diabatic formalism: Charge transfer in the ethylene dimer cation and excited state dynamics in the 2-pyridone dimer. Journal of Chemical Physics, 2012, 137, 22A514. | 1.2 | 173 |

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| 19 | Columbusâ€”a program system for advanced multireference theory calculations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 191-199. | 6.2 | 171 |
| 20 | Surface Hopping Dynamics with Correlated Single-Reference Methods: 9H-Adenine as a Case Study. Journal of Chemical Theory and Computation, 2014, 10, 1395-1405. | 2.3 | 170 |
| 21 | Solvent Effects on Hydrogen BondsA Theoretical Study. Journal of Physical Chemistry A, 2002, 106, 1862-1871. | 1.1 | 167 |
| 22 | Ab Initio Molecular Dynamics Study of a Monomolecular Water Layer on Octahedral and Tetrahedral Kaolinite Surfaces. Journal of Physical Chemistry B, 2004, 108, 5930-5936. | 1.2 | 146 |
| 23 | Implementation of an electronic structure program system on the CYBER 205. Journal of Computational Chemistry, 1985, 6, 200-208. | 1.5 | 143 |
| 24 | Ab initio investigation on the lowest singlet and triplet state of disilyne (Si2H2). Journal of the American Chemical Society, 1983, 105, 6646-6649. | 6.6 | 142 |
| 25 | Theoretical Study of Vibrational and Optical Spectra of Methylene-Bridged Oligofluorenes. Journal of Physical Chemistry A, 2005, 109, 10232-10238. | 1.1 | 129 |
| 26 | Non-adiabatic dynamics of pyrrole: Dependence of deactivation mechanisms on the excitation energy. Chemical Physics, 2010, 375, 26-34. | 0.9 | 124 |
| 27 | Structure and stability of the carbocations C2H3+ and C2H4X+, X = hydrogen, fluorine, chlorine, and methyl. Ab initio investigation including electron correlation and a comparison with MINDO/3 results. Journal of the American Chemical Society, 1978, 100, 5297-5305. | 6.6 | 120 |
| 28 | Rotational Barrier in Phenalenyl Neutral Radical Dimer: Separating Pancake and van der Waals Interactions. Journal of the American Chemical Society, 2014, 136, 5539-5542. | 6.6 | 120 |
| 29 | A systematic theoretical investigation of the valence excited states of the diatomic molecules B 2 , C 2 , N 2 and O 2. Theoretical Chemistry Accounts, 2001, 105, 227-243. | 0.5 | 110 |
| 30 | Excited-State Diproton Transfer in [2,2â€²-Bipyridyl]-3,3â€²-diol: the Mechanism Is Sequential, Not Concerted. Journal of Physical Chemistry A, 2009, 113, 8490-8499. | 1.1 | 110 |
| 31 | Nonadiabatic Molecular Dynamics Study of the cisâ€“trans Photoisomerization of Azobenzene Excited to the S<sub>1</sub> State. Journal of Physical Chemistry A, 2011, 115, 11136-11143. | 1.1 | 109 |
| 32 | Theoretical Study of Adsorption Sites on the (001) Surfaces of 1:1 Clay Minerals. Langmuir, 2002, 18, 139-147. | 1.6 | 106 |
| 33 | Optimization of mixed quantum-classical dynamics: Time-derivative coupling terms and selected couplings. Chemical Physics, 2009, 356, 147-152. | 0.9 | 106 |
| 34 | Ab Initio Molecular Dynamics Study of Adsorption Sites on the (001) Surfaces of 1:1 Dioctahedral Clay Minerals. Journal of Physical Chemistry B, 2002, 106, 11515-11525. | 1.2 | 105 |
| 35 | Coupled pair functional study on the hydrogen fluoride dimer. I. Energy surface and characterization of stationary points. Chemical Physics, 1988, 121, 137-153. | 0.9 | 102 |
| 36 | Critical appraisal of excited state nonadiabatic dynamics simulations of 9H-adenine. Journal of Chemical Physics, 2012, 137, 22A503. | 1.2 | 102 |

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| 37 | The nonadiabatic deactivation paths of pyrrole. Journal of Chemical Physics, 2006, 125, 164323. | 1.2 | 101 |
| 38 | Automerization reaction of cyclobutadiene and its barrier height: Anab initiobenchmark multireference average-quadratic coupled cluster study. Journal of Chemical Physics, 2006, 125, 064310. | 1.2 | 101 |
| 39 | Theoretical investigations on carbocations. Structure and stability of C3H5+,C4H9+(2-butyl cation), C5H5+,C6H7+(protonated benzene), and C7H11+(2-norbornyl cation). Journal of the American Chemical Society, 1979, 101, 3479-3486. | 6.6 | 92 |
| 40 | The interplay of skeletal deformations and ultrafast excited-state intramolecular proton transfer: Experimental and theoretical investigation of 10-hydroxybenzo[h]quinoline. Chemical Physics, 2008, 347, 446-461. | 0.9 | 91 |
| 41 | Polyradical Character of Triangular Non-KekulÃ© Structures, Zethrenes, p-Quinodimethane-Linked Bisphenalenyl, and the Clar Goblet in Comparison: An Extended Multireference Study. Journal of Physical Chemistry A, 2016, 120, 1625-1636. | 1.1 | 91 |
| 42 | Ab initio calculations on intermolecular forces. III. Effect of electron correlation on the hydrogen bond in the hydrofluoric acid dimer. Journal of the American Chemical Society, 1974, 96, 4761-4766. | 6.6 | 87 |
| 43 | An analytical sixâ€dimensional potential energy surface for (HF)2 from ab initio calculations. Journal of Chemical Physics, 1988, 89, 3002-3007. | 1.2 | 87 |
| 44 | The ethylene 1â€Š1B1uâ€Šv state revisited. Journal of Chemical Physics, 1999, 110, 7176-7184. | 1.2 | 86 |
| 45 | Photodynamics Simulations of Thymine: Relaxation into the First Excited Singlet State. Journal of Physical Chemistry A, 2009, 113, 12686-12693. | 1.1 | 85 |
| 46 | Photodynamical simulations of cytosine: characterization of the ultrafast bi-exponential UV deactivation. Physical Chemistry Chemical Physics, 2011, 13, 6145. | 1.3 | 84 |
| 47 | Nonadiabatic Dynamics of Uracil: Population Split among Different Decay Mechanisms. Journal of Physical Chemistry A, 2011, 115, 5247-5255. | 1.1 | 84 |
| 48 | Ab initio studies on hydrogen-bonded clusters. I. Linear and cyclic oligomers of hydrogen cyanide. Chemical Physics, 1987, 113, 53-64. | 0.9 | 83 |
| 49 | Ab initio studies on heterocyclic conjugated polymers: structure and vibrational spectra of thiophene, oligothiophenes and polythiophene. Computational and Theoretical Chemistry, 1992, 259, 181-198. | 1.5 | 83 |
| 50 | Nonadiabatic excited-state dynamics of polar Ï€-systems and related model compounds of biological relevance. Physical Chemistry Chemical Physics, 2008, 10, 482-494. | 1.3 | 80 |
| 51 | Electronically excited states and photodynamics: a continuing challenge. Theoretical Chemistry Accounts, 2012, 131, 1. | 0.5 | 77 |
| 52 | A systematic investigation on the structure and stability of the lowest singlet and triplet states of Si2H4 and SiH3SiH and the carbon analogous compounds SiH2CH2, SiH3CH, CH3SiH, C2H4, and CH3CH. Journal of the American Chemical Society, 1982, 104, 5884-5889. | 6.6 | 75 |
| 53 | Nonadiabatic Excited-State Dynamics with Hybrid ab Initio Quantum-Mechanical/Molecular-Mechanical Methods: Solvation of the Pentadieniminium Cation in Apolar Media. Journal of Physical Chemistry A, 2010, 114, 6757-6765. | 1.1 | 74 |
| 54 | Double Pancake Bonds: Pushing the Limits of Strong Ï€â€“Ï€ Stacking Interactions. Journal of the American Chemical Society, 2014, 136, 12958-12965. | 6.6 | 74 |

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| 55 | Electronic structure and proton affinity of methylenephosphorane by ab initio methods including electron correlation. Journal of the American Chemical Society, 1977, 99, 353-360. | 6.6 | 73 |
| 56 | Ab initio calculations on the excited states of Ï€-systems. I. Valence excitations in acetylene. Chemical Physics, 1986, 102, 77-89. | 0.9 | 73 |
| 57 | The chargeâ€transfer states in a stacked nucleobase dimer complex: A benchmark study. Journal of Computational Chemistry, 2011, 32, 1217-1227. | 1.5 | 73 |
| 58 | Ab initio studies on heterocyclic conjugated polymers: Structure and vibrational spectra of pyrrole, oligopyrroles, and polypyrrole. Journal of Chemical Physics, 1992, 96, 4464-4473. | 1.2 | 70 |
| 59 | The decay mechanism of photoexcited guanine â˜… A nonadiabatic dynamics study. Journal of Chemical Physics, 2011, 134, 014304. | 1.2 | 70 |
| 60 | UV Absorption Spectrum of Alternating DNA Duplexes. Analysis of Excitonic and Charge Transfer Interactions. Journal of Physical Chemistry A, 2012, 116, 11151-11160. | 1.1 | 70 |
| 61 | A massively parallel multireference configuration interaction program: The parallel COLUMBUS program. Journal of Computational Chemistry, 1997, 18, 430-448. | 1.5 | 69 |
| 62 | Spectral broadening and diffusion by torsional motion in biphenyl. Journal of Chemical Physics, 2005, 123, 144311. | 1.2 | 69 |
| 63 | The effect of hydrogen bonding on the excited-state proton transfer in 2-(2â€²-hydroxyphenyl)benzothiazole: a TDDFT molecular dynamics study. Physical Chemistry Chemical Physics, 2012, 14, 9016. | 1.3 | 69 |
| 64 | An ab initio calculation of the intramolecular stretching spectra for the HF dimer and its Dâ€substituted isotopic species. Journal of Chemical Physics, 1990, 93, 6266-6280. | 1.2 | 68 |
| 65 | Excitation energies and transition moments by the multireference averaged quadratic coupled cluster (MR-AQCC) method. Physical Chemistry Chemical Physics, 2000, 2, 2067-2073. | 1.3 | 68 |
| 66 | New implementation of the graphical unitary group approach for multireference direct configuration interaction calculations. International Journal of Quantum Chemistry, 1981, 20, 91-100. | 1.0 | 68 |
| 67 | Can the Nonadiabatic Photodynamics of Aminopyrimidine Be a Model for the Ultrafast Deactivation of Adenine?. Journal of Physical Chemistry A, 2007, 111, 2852-2858. | 1.1 | 67 |
| 68 | Does Stacking Restrain the Photodynamics of Individual Nucleobases?. Journal of the American Chemical Society, 2010, 132, 8261-8263. | 6.6 | 67 |
| 69 | Excited-state non-adiabatic dynamics simulations of pyrrole. Molecular Physics, 2009, 107, 845-854. | 0.8 | 65 |
| 70 | Electronically Excited States in Poly(p-phenylenevinylene): Vertical Excitations and Torsional Potentials from High-Level Ab Initio Calculations. Journal of Physical Chemistry A, 2013, 117, 2181-2189. | 1.1 | 65 |
| 71 | Ultrafast two-step process in the non-adiabatic relaxation of the CH2 molecule. Molecular Physics, 2006, 104, 1053-1060. | 0.8 | 64 |
| 72 | A note on the AB initio calculation of intermolecular potentials: the HF dimer. Chemical Physics Letters, 1979, 66, 108-110. | 1.2 | 63 |

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| 73 | An ab initio calculation of the stretching energies for the HF dimer. Journal of Chemical Physics, 1990, 92, 7432-7440. | 1.2 | 62 |
| 74 | Excited State Properties of 7-Hydroxy-4-methylcoumarin in the Gas Phase and in Solution. A Theoretical Study. Journal of Physical Chemistry A, 2005, 109, 11860-11869. | 1.1 | 62 |
| 75 | Dependence of Optical Properties of Oligo-para-phenylenes on Torsional Modes and Chain Length. Journal of Physical Chemistry B, 2007, 111, 7954-7962. | 1.2 | 62 |
| 76 | Intramolecular Charge-Transfer Excited-State Processes in 4-(N,N-Dimethylamino)benzonitrile: The Role of Twisting and the Ï€Ïƒ* State. Journal of Physical Chemistry A, 2015, 119, 6232-6243. | 1.1 | 60 |
| 77 | An ab initio semirigid bender calculation of the rotation and transâ€tunneling spectra of (HF)2 and (DF)2. Journal of Chemical Physics, 1989, 91, 5154-5159. | 1.2 | 59 |
| 78 | Ab Initio Modeling of Excitonic and Charge-Transfer States in Organic Semiconductors: The PTB1/PCBM Low Band Gap System. Journal of the American Chemical Society, 2013, 135, 18252-18255. | 6.6 | 59 |
| 79 | UV excitation and radiationless deactivation of imidazole. Journal of Chemical Physics, 2009, 130, 034305. | 1.2 | 58 |
| 80 | On the structure and stability of singlet and triplet disilene and silylsilylene. Chemical Physics Letters, 1982, 85, 467-471. | 1.2 | 57 |
| 81 | Bridged structures in multiply bonded silicon compounds: Disilyne, protonated disilyne and disilene. Chemical Physics Letters, 1984, 112, 33-40. | 1.2 | 57 |
| 82 | Ï€â€“Ï€ stacking between polyaromatic hydrocarbon sheets beyond dispersion interactions. Physical Chemistry Chemical Physics, 2016, 18, 22300-22310. | 1.3 | 57 |
| 83 | Progress and challenges in understanding of photoluminescence properties of carbon dots based on theoretical computations. Applied Materials Today, 2021, 22, 100924. | 2.3 | 57 |
| 84 | A comparison of singlet and triplet states for one- and two-dimensional graphene nanoribbons using multireference theory. Theoretical Chemistry Accounts, 2014, 133, 1. | 0.5 | 56 |
| 85 | Nonadiabatic Photodynamics of a Retinal Model in Polar and Nonpolar Environment. Journal of Physical Chemistry A, 2013, 117, 2790-2799. | 1.1 | 55 |
| 86 | Ab initio calculations on small hydrides including electron correlation. Theoretica Chimica Acta, 1973, 31, 39-48. | 0.9 | 54 |
| 87 | Dynamics starting at a conical intersection: Application to the photochemistry of pyrrole. Journal of Chemical Physics, 2009, 131, 024312. | 1.2 | 54 |
| 88 | Molecular Dynamics Simulations of Water Molecule-Bridges in Polar Domains of Humic Acids. Environmental Science & Technology, 2011, 45, 8411-8419. | 4.6 | 54 |
| 89 | Comparison of LC-TDDFT and ADC(2) Methods in Computations of Bright and Charge Transfer States in Stacked Oligothiophenes. Journal of Chemical Theory and Computation, 2014, 10, 3280-3289. | 2.3 | 54 |
| 90 | A systematic ab initio investigation of the open and ring structures of ozone. Chemical Physics Letters, 1998, 293, 72-80. | 1.2 | 53 |

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| 91 | Combined ab initio and density functional study on polaron to bipolaron transitions in oligophenyls and oligothiophenes. Journal of Chemical Physics, 1997, 107, 3021-3031. | 1.2 | 52 |
| 92 | Acidâ€“base properties of a goethite surface model: A theoretical view. Geochimica Et Cosmochimica Acta, 2008, 72, 3587-3602. | 1.6 | 50 |
| 93 | The Dielsâ€“Alder Reaction of Ethene and 1,3-Butadiene: An Extended Multireference ab initio Investigation. ChemPhysChem, 2004, 5, 1365-1371. | 1.0 | 47 |
| 94 | Stabilizing Capacity of Water Bridges in Nanopore Segments of Humic Substances: A Theoretical Investigation. Journal of Physical Chemistry C, 2009, 113, 16468-16475. | 1.5 | 47 |
| 95 | Solvent effects in electronically excited states using the continuum solvation model COSMO in combination with multireference configuration interaction with singles and doubles (MR-CISD). Theoretical Chemistry Accounts, 2004, 111, 78-89. | 0.5 | 46 |
| 96 | Simulation of the photodeactivation of formamide in the nO-Ï€âˆ— and Ï€-Ï€âˆ— states: An ab initio on-the-fly surface-hopping dynamics study. Journal of Chemical Physics, 2007, 127, 234303. | 1.2 | 46 |
| 97 | The functionality of cation bridges for binding polar groups in soil aggregates. International Journal of Quantum Chemistry, 2011, 111, 1531-1542. | 1.0 | 46 |
| 98 | Electronic excitation and structural relaxation of the adenine dinucleotide in gas phase and solution. Photochemical and Photobiological Sciences, 2013, 12, 1440-1452. | 1.6 | 46 |
| 99 | Anabinitioinvestigation of the chargeâ€transfer complexes of alkali atoms with oligo (Î±,Î±â€²) thiophenes and oligoparaphenylenes: A model calculation on polaronic and bipolaronic defect structures. Journal of Chemical Physics, 1995, 103, 1508-1522. | 1.2 | 45 |
| 100 | Response of sorption processes of MCPA to the amount and origin of organic matter in a long-term field experiment. European Journal of Soil Science, 2001, 52, 279-286. | 1.8 | 45 |
| 101 | The valence-excited states T1â€“T4 and S1â€“S2 of acetylene: A high-level MR-CISD and MR-AQCC investigation of stationary points, potential energy surfaces, and surface crossings. Journal of Chemical Physics, 2003, 118, 1702-1713. | 1.2 | 45 |
| 102 | An extended multireference study of the electronic states of para-benzyne. Journal of Chemical Physics, 2008, 129, 044306. | 1.2 | 45 |
| 103 | Excited-State Intermolecular Proton Transfer Reactions of 7-Azaindole(MeOH)<sub>n</sub> (n = 1â€“3) Clusters in the Gas phase: On-the-Fly Dynamics Simulation. Journal of Physical Chemistry A, 2011, 115, 14129-14136. | 1.1 | 45 |
| 104 | Interaction of Acetate Anion with Hydrated Al3+Cation:Â A Theoretical Study. Journal of Physical Chemistry A, 2000, 104, 6824-6833. | 1.1 | 44 |
| 105 | A systematic theoretical investigation of the lowest valence- and Rydberg-excited singlet states of trans-butadiene. The character of the 1 1 B u (V) state revisited. Theoretical Chemistry Accounts, 2004, 112, 16-26. | 0.5 | 44 |
| 106 | A parallel implementation of the COLUMBUS multireference configuration interaction program. Theoretica Chimica Acta, 1993, 84, 489-509. | 0.9 | 43 |
| 107 | Excited-State Properties and Environmental Effects for Protonated Schiff Bases: A Theoretical Study. ChemPhysChem, 2006, 7, 2089-2096. | 1.0 | 43 |
| 108 | Excited-State Proton Transfer in 7-Hydroxy-4-methylcoumarin along a Hydrogen-Bonded Water Wire. Journal of Physical Chemistry A, 2007, 111, 127-135. | 1.1 | 43 |

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| 109 | Azomethane: Nonadiabatic Photodynamical Simulations in Solution. Journal of Physical Chemistry A, 2010, 114, 12585-12590. | 1.1 | 43 |
| 110 | Absorption and Fluorescence of PRODAN in Phospholipid Bilayers: A Combined Quantum Mechanics and Classical Molecular Dynamics Study. Journal of Physical Chemistry A, 2011, 115, 11428-11437. | 1.1 | 43 |
| 111 | Study of the Diradicaloid Character in a Prototypical Pancakeâ€Bonded Dimer: The Stacked Tetracyanoethylene (TCNE) Anion Dimer and the Neutral K<sub>2</sub>TCNE<sub>2</sub> Complex. ChemPhysChem, 2014, 15, 165-176. | 1.0 | 43 |
| 112 | Intermolecular interactions and charge transfer transitions in aromatic hydrocarbonâ€“tetracyanoethylene complexes. Physical Chemistry Chemical Physics, 2014, 16, 20586-20597. | 1.3 | 43 |
| 113 | The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110. | 1.2 | 42 |
| 114 | A density-functional investigation of aluminium(III)â€“citrate complexes. Physical Chemistry Chemical Physics, 2001, 3, 1979-1985. | 1.3 | 41 |
| 115 | Determination of energy minima and saddle points using multireference configuration interaction methods in combination with reduced gradient following: The S0 surface of H2CO and the T1 and T2 surfaces of acetylene. Journal of Computational Chemistry, 2002, 23, 576-583. | 1.5 | 41 |
| 116 | A Multireference Configuration Interaction Investigation of the Excited-State Energy Surfaces of Fluoroethylene (C2H3F). Journal of Physical Chemistry A, 2005, 109, 5168-5175. | 1.1 | 41 |
| 117 | Ultrafast non-adiabatic dynamics of ethylene including Rydberg states. Molecular Physics, 2013, 111, 2439-2450. | 0.8 | 41 |
| 118 | Linear versus cyclic (HCN)3: An ab initio study on structure, vibrational spectra, and infrared intensities. Journal of Chemical Physics, 1990, 92, 2469-2477. | 1.2 | 40 |
| 119 | From butadiene to polyacetylene: An ab initio study on the vibrational spectra of polyenes. Journal of Chemical Physics, 1992, 96, 982-996. | 1.2 | 40 |
| 120 | Ab initio nonadiabatic dynamics study of ultrafast radiationless decay over conical intersections illustrated on the Na3F cluster. Journal of Chemical Physics, 2006, 125, 024303. | 1.2 | 40 |
| 121 | Interaction of the 2,4-dichlorophenoxyacetic acid herbicide with soil organic matter moieties: a theoretical study. European Journal of Soil Science, 2007, 58, 889-899. | 1.8 | 40 |
| 122 | Concave or convex Ï€-dimers: the role of the pancake bond in substituted phenalenyl radical dimers. Physical Chemistry Chemical Physics, 2015, 17, 23963-23969. | 1.3 | 40 |
| 123 | Adsorption of organic substances on broken clay surfaces: A quantum chemical study. Journal of Computational Chemistry, 2003, 24, 1853-1863. | 1.5 | 39 |
| 124 | Quantum Chemical Adsorption Studies on the (110) Surface of the Mineral Goethite. Journal of Physical Chemistry C, 2007, 111, 877-885. | 1.5 | 39 |
| 125 | Is the Photoinduced Isomerization in Retinal Protonated Schiff Bases a Single- or Double-Torsional Process?. Journal of Physical Chemistry A, 2009, 113, 11907-11918. | 1.1 | 39 |
| 126 | Geometry optimization of excited valence states of formaldehyde using analytical multireference configuration interaction singles and doubles and multireference averaged quadratic coupled-cluster gradients, and the conical intersection formed by the 1â€Š[sup 1]B[sub 1](Ïƒ-Ï€[sup â^—]) and 2â€Š[sup 1]A[sub 1](Ï€-Ï€[sup â^—]) states. Journal of Chemical Physics, 2001, 114, 746. | 1.2 | 38 |

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| 127 | The thermodynamic stability of hydrogen bonded and cation bridged complexes of humic acid modelsâ€"A theoretical study. Chemical Physics, 2008, 349, 69-76. | 0.9 | 37 |
| 128 | Model study on sorption of polycyclic aromatic hydrocarbons to goethite. Journal of Colloid and Interface Science, 2009, 330, 244-249. | 5.0 | 37 |
| 129 | Modeling Catalytic Effects of Clay Mineral Surfaces on Peptide Bond Formation. Journal of Physical Chemistry B, 2004, 108, 10120-10130. | 1.2 | 36 |
| 130 | High-level theoretical benchmark investigations of the UV-vis absorption spectra of paradigmatic polycyclic aromatic hydrocarbons as models for graphene quantum dots. Journal of Chemical Physics, 2019, 150, 124302. | 1.2 | 35 |
| 131 | Photodynamics of Azomethane: A Nonadiabatic Surface-Hopping Study<sup>â€</sup>. Journal of Physical Chemistry A, 2010, 114, 8778-8785. | 1.1 | 34 |
| 132 | Excited states and excitonic interactions in prototypic polycyclic aromatic hydrocarbon dimers as models for graphitic interactions in carbon dots. Physical Chemistry Chemical Physics, 2019, 21, 9077-9088. | 1.3 | 34 |
| 133 | Perturbational treatment of spin-orbit coupling for generally applicable high-level multi-reference methods. Journal of Chemical Physics, 2014, 141, 074105. | 1.2 | 33 |
| 134 | Diradical Organic Oneâ€Dimensional Polymers Synthesized on a Metallic Surface. Angewandte Chemie - International Edition, 2020, 59, 17594-17599. | 7.2 | 33 |
| 135 | Mechanism of Ultrafast Photodecay in Restricted Motions in Protonated Schiff Bases: The Pentadieniminium Cation. Journal of Chemical Theory and Computation, 2008, 4, 1189-1199. | 2.3 | 32 |
| 136 | Strikingly Different Effects of Hydrogen Bonding on the Photodynamics of Individual Nucleobases in DNA: Comparison of Guanine and Cytosine. Journal of the American Chemical Society, 2012, 134, 13662-13669. | 6.6 | 31 |
| 137 | New Insights into the State Trapping of UV-Excited Thymine. Molecules, 2016, 21, 1603. | 1.7 | 31 |
| 138 | A density functional theoretical study on solvated Al3+â€"oxalate complexes: structures and thermodynamic properties. Physical Chemistry Chemical Physics, 2000, 2, 2845-2850. | 1.3 | 30 |
| 139 | Multiple pathways in the photodynamics of a polar Ï€-bond: A case study of silaethylene. Chemical Physics Letters, 2006, 418, 377-382. | 1.2 | 30 |
| 140 | Singlet L<sub>a</sub> and L<sub>b</sub> Bands for N-Acenes (N = 2â€"7): A CASSCF/CASPT2 Study. Journal of Chemical Theory and Computation, 2017, 13, 4297-4306. | 2.3 | 30 |
| 141 | AB initio calculations on intermolecular forces. The systems Heâ€¦HF and Heâ€¦H2O. Chemical Physics Letters, 1973, 20, 448-453. | 1.2 | 29 |
| 142 | Effect of substituents on the excited-state dynamics of the modified DNA bases 2,4-diaminopyrimidine and 2,6-diaminopurine. Physical Chemistry Chemical Physics, 2010, 12, 5375. | 1.3 | 29 |
| 143 | Matrix-controlled photofragmentation of formamide: dynamics simulation in argon by nonadiabatic QM/MM method. Physical Chemistry Chemical Physics, 2010, 12, 12719. | 1.3 | 29 |
| 144 | Ab initio calculations including electron correlation, and mindo/3 calculations on the system C2H+7. Chemical Physics Letters, 1978, 58, 175-179. | 1.2 | 28 |

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| 145 | Why water makes 2-aminopurine fluorescent?. Physical Chemistry Chemical Physics, 2015, 17, 15452-15459. | 1.3 | 28 |
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