Hans Lischka

List of Publications by Citations

318 papers	14,286 citations	61 h-index	107 g-index
323 ext. papers	15,438 ext. citations	4.4 avg, IF	6.51 L-index

#	Paper	IF	Citations
318	Molcas 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. *Journal of Computational Chemistry*, **2016**, 37, 506-41	3.5	1047
317	Multiconfiguration self-consistent field and multireference configuration interaction methods and applications. *Chemical Reviews*, **2012**, 112, 108-81	68.1	462
316	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 spin□orbit CI and parallel CI density. *Physical Chemistry Chemical Physics*, **2001**, 3, 664-673	3.6	369
315	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	4.7	366
314	A progress report on the status of the COLUMBUS MRCI program system. *International Journal of Quantum Chemistry*, **1988**, 34, 149-165	2.1	343
313	Relaxation mechanisms of UV-photoexcited DNA and RNA nucleobases. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 21453-8	11.5	323
312	Analysis of Excitonic and Charge Transfer Interactions from Quantum Chemical Calculations. *Journal of Chemical Theory and Computation*, **2012**, 8, 2777-89	6.4	284
311	Newton-X: a surface-hopping program for nonadiabatic molecular dynamics. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 26-33	7.9	280
310	Analytic evaluation of nonadiabatic coupling terms at the MR-CI level. I. Formalism. *Journal of Chemical Physics*, **2004**, 120, 7322-9	3.9	270
309	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, 7330-9	3.9	208
308	Multireference Approaches for Excited States of Molecules. *Chemical Reviews*, **2018**, 118, 7293-7361	68.1	181
307	The UV absorption of nucleobases: semi-classical ab initio spectra simulations. *Physical Chemistry Chemical Physics*, **2010**, 12, 4959-67	3.6	179
306	Nonadiabatic deactivation of 9H-adenine: a comprehensive picture based on mixed quantum-classical dynamics. *Journal of the American Chemical Society*, **2008**, 130, 6831-9	16.4	178
305	The multiradical character of one- and two-dimensional graphene nanoribbons. *Angewandte Chemie - International Edition*, **2013**, 52, 2581-4	16.4	168
304	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
303	Ultrafast internal conversion pathway and mechanism in 2-(2Phydroxyphenyl)benzothiazole: a case study for excited-state intramolecular proton transfer systems. *Physical Chemistry Chemical Physics*, **2009**, 11, 1406-15	3.6	154
302	Columbus□ program system for advanced multireference theory calculations. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 191-199	7.9	147

301	Solvent Effects on Hydrogen BondsA Theoretical Study. *Journal of Physical Chemistry A*, **2002**, 106, 1862-1871	2.8	145
300	Implementation of an electronic structure program system on the CYBER 205. *Journal of Computational Chemistry*, **1985**, 6, 200-208	3.5	143
299	Surface Hopping Dynamics with Correlated Single-Reference Methods: 9H-Adenine as a Case Study. *Journal of Chemical Theory and Computation*, **2014**, 10, 1395-405	6.4	139
298	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	3.9	139
297	Ab initio investigation on the lowest singlet and triplet state of disilyne (Si2H2). *Journal of the American Chemical Society*, **1983**, 105, 6646-6649	16.4	131
296	Wettability of kaolinite (001) surfaces Molecular dynamic study. *Geoderma*, **2011**, 169, 47-54	6.7	128
295	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	3.4	118
294	Non-adiabatic dynamics of pyrrole: Dependence of deactivation mechanisms on the excitation energy. *Chemical Physics*, **2010**, 375, 26-34	2.3	115
293	Theoretical study of vibrational and optical spectra of methylene-bridged oligofluorenes. *Journal of Physical Chemistry A*, **2005**, 109, 10232-8	2.8	106
292	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	16.4	106
291	A systematic theoretical investigation of the valence excited states of the diatomic molecules B2, C2, N2 and O2. *Theoretical Chemistry Accounts*, **2001**, 105, 227-243	1.9	102
290	Rotational barrier in phenalenyl neutral radical dimer: separating pancake and van der Waals interactions. *Journal of the American Chemical Society*, **2014**, 136, 5539-42	16.4	101
289	The nonadiabatic deactivation paths of pyrrole. *Journal of Chemical Physics*, **2006**, 125, 164323	3.9	99
288	Theoretical Study of Adsorption Sites on the (001) Surfaces of 1:1 Clay Minerals. *Langmuir*, **2002**, 18, 139-147	4	99
287	Nonadiabatic molecular dynamics study of the cis-trans photoisomerization of azobenzene excited to the S1 state. *Journal of Physical Chemistry A*, **2011**, 115, 11136-43	2.8	97
286	Coupled pair functional study on the hydrogen fluoride dimer. I. Energy surface and characterization of stationary points. *Chemical Physics*, **1988**, 121, 137-153	2.3	97
285	Excited-state diproton transfer in [2,2Pbipyridyl]-3,3Pdiol: the mechanism is sequential, not concerted. *Journal of Physical Chemistry A*, **2009**, 113, 8490-9	2.8	96
284	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	3.4	95

283	Critical appraisal of excited state nonadiabatic dynamics simulations of 9H-adenine. *Journal of Chemical Physics*, **2012**, 137, 22A503	3.9	90
282	Optimization of mixed quantum-classical dynamics: Time-derivative coupling terms and selected couplings. *Chemical Physics*, **2009**, 356, 147-152	2.3	90
281	Automerization reaction of cyclobutadiene and its barrier height: an ab initio benchmark multireference average-quadratic coupled cluster study. *Journal of Chemical Physics*, **2006**, 125, 64310	3.9	87
280	An analytical six-dimensional potential energy surface for (HF)2 from ab initio calculations. *Journal of Chemical Physics*, **1988**, 89, 3002-3007	3.9	85
279	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	16.4	83
278	Photodynamics simulations of thymine: relaxation into the first excited singlet state. *Journal of Physical Chemistry A*, **2009**, 113, 12686-93	2.8	82
277	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	2.3	82
276	The ethylene 1 1B1u V state revisited. *Journal of Chemical Physics*, **1999**, 110, 7176-7184	3.9	80
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274	Photodynamical simulations of cytosine: characterization of the ultrafast bi-exponential UV deactivation. *Physical Chemistry Chemical Physics*, **2011**, 13, 6145-55	3.6	79
273	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	16.4	79
272	Nonadiabatic dynamics of uracil: population split among different decay mechanisms. *Journal of Physical Chemistry A*, **2011**, 115, 5247-55	2.8	77
271	Nonadiabatic excited-state dynamics of polar pi-systems and related model compounds of biological relevance. *Physical Chemistry Chemical Physics*, **2008**, 10, 482-94	3.6	76
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269	Ab initio calculations on the excited states of □ systems. I. Valence excitations in acetylene. *Chemical Physics*, **1986**, 102, 77-89	2.3	72
268	Polyradical Character of Triangular Non-Kekul□ Structures, Zethrenes, p-Quinodimethane-Linked Bisphenalenyl, and the Clar Goblet in Comparison: An Extended Multireference Study. *Journal of Physical Chemistry A*, **2016**, 120, 1625-36	2.8	70
267	Electronically excited states and photodynamics: a continuing challenge. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	69
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255	Excitation energies and transition moments by the multireference averaged quadratic coupled cluster (MR-AQCC) method. *Physical Chemistry Chemical Physics*, **2000**, 2, 2067-2073	3.6	61
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253	Electronic structure and proton affinity of methylenephosphorane by ab initio methods including electron correlation. *Journal of the American Chemical Society*, **1977**, 99, 353-360	16.4	61
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234	Dynamics starting at a conical intersection: application to the photochemistry of pyrrole. *Journal of Chemical Physics*, **2009**, 131, 024312	3.9	48
233	Acid–Base properties of a goethite surface model: A theoretical view. *Geochimica Et Cosmochimica Acta*, **2008**, 72, 3587-3602	5.5	48
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224	Electronic excitation and structural relaxation of the adenine dinucleotide in gas phase and solution. *Photochemical and Photobiological Sciences*, **2013**, 12, 1440-52	4.2	43
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