Roland H Lindh

List of Publications by Citations

220 papers	15,736 citations	58 h-index	122 g-index
241 ext. papers	17,198 ext. citations	4.9 avg, IF	6.42 L-index

#	Paper	IF	Citations
220	MOLCAS: a program package for computational chemistry. *Computational Materials Science*, **2003**, 28, 222-239	3.2	1617
219	MOLCAS 7: the next generation. *Journal of Computational Chemistry*, **2010**, 31, 224-47	3.5	1425
218	Molcas 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. *Journal of Computational Chemistry*, **2016**, 37, 506-41	3.5	1047
217	Main Group Atoms and Dimers Studied with a New Relativistic ANO Basis Set. *Journal of Physical Chemistry A*, **2004**, 108, 2851-2858	2.8	1020
216	New relativistic ANO basis sets for transition metal atoms. *Journal of Physical Chemistry A*, **2005**, 109, 6575-9	2.8	799
215	Towards an accurate molecular orbital theory for excited states: Ethene, butadiene, and hexatriene. *Journal of Chemical Physics*, **1993**, 98, 3151-3162	3.9	380
214	OpenMolcas: From Source Code to Insight. *Journal of Chemical Theory and Computation*, **2019**, 15, 5925-5964	5.4	310
213	New relativistic atomic natural orbital basis sets for lanthanide atoms with applications to the Ce diatom and LuF3. *Journal of Physical Chemistry A*, **2008**, 112, 11431-5	2.8	296
212	2MOLCAS as a development platform for quantum chemistry software. *International Journal of Quantum Chemistry*, **2004**, 100, 626-635	2.1	293
211	Local properties of quantum chemical systems: the LoProp approach. *Journal of Chemical Physics*, **2004**, 121, 4494-500	3.9	282
210	Low-cost evaluation of the exchange Fock matrix from Cholesky and density fitting representations of the electron repulsion integrals. *Journal of Chemical Physics*, **2007**, 126, 194106	3.9	256
209	The reduced multiplication scheme of the Rys quadrature and new recurrence relations for auxiliary function based two-electron integral evaluation. *Journal of Chemical Physics*, **1991**, 95, 5889-5897	3.9	235
208	Unbiased auxiliary basis sets for accurate two-electron integral approximations. *Journal of Chemical Physics*, **2007**, 127, 114107	3.9	228
207	New relativistic ANO basis sets for actinide atoms. *Chemical Physics Letters*, **2005**, 409, 295-299	2.5	220
206	Analytical energy gradients for local second-order Møller-Plesset perturbation theory using density fitting approximations. *Journal of Chemical Physics*, **2004**, 121, 737-50	3.9	206
205	Chemi- and Bioluminescence of Cyclic Peroxides. *Chemical Reviews*, **2018**, 118, 6927-6974	68.1	172
204	Theoretical Study of the Internal Charge Transfer in Aminobenzonitriles. *Journal of the American Chemical Society*, **1995**, 117, 3189-3204	16.4	170

203	Atomic Cholesky decompositions: a route to unbiased auxiliary basis sets for density fitting approximation with tunable accuracy and efficiency. *Journal of Chemical Physics*, **2009**, 130, 154107	3.9	160
202	Accurate ab initio density fitting for multiconfigurational self-consistent field methods. *Journal of Chemical Physics*, **2008**, 129, 024113	3.9	145
201	Multiconfiguration second-order perturbation theory approach to strong electron correlation in chemistry and photochemistry. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 585-603	7.9	143
200	The ultrafast photoisomerizations of rhodopsin and bathorhodopsin are modulated by bond length alternation and HOOP driven electronic effects. *Journal of the American Chemical Society*, **2011**, 133, 3354-64	16.4	139
199	Shape of Multireference, Equation-of-Motion Coupled-Cluster, and Density Functional Theory Potential Energy Surfaces at a Conical Intersection. *Journal of Chemical Theory and Computation*, **2014**, 10, 3074-84	6.4	132
198	Dynamic Electron Correlation Effects on the Ground State Potential Energy Surface of a Retinal Chromophore Model. *Journal of Chemical Theory and Computation*, **2012**, 8, 4069-80	6.4	127
197	Density fitting with auxiliary basis sets from Cholesky decompositions. *Theoretical Chemistry Accounts*, **2009**, 124, 1-10	1.9	123
196	Theoretical study of the electronic spectrum of all-trans-1,3,5,7-octatetraene. *The Journal of Physical Chemistry*, **1993**, 97, 9360-9368		122
195	Computation of conical intersections by using perturbation techniques. *Journal of Chemical Physics*, **2005**, 122, 104107	3.9	107
194	Modern quantum chemistry with [Open]Molcas. *Journal of Chemical Physics*, **2020**, 152, 214117	3.9	106
193	The water dimer interaction energy: Convergence to the basis set limit at the correlated level. *Journal of Chemical Physics*, **1997**, 107, 4597-4605	3.9	106
192	Extended ab Initio and Theoretical Thermodynamics Studies of the Bergman Reaction and the Energy Splitting of the Singlet o-, m-, and p-Benzynes. *Journal of the American Chemical Society*, **1995**, 117, 7186-7194	16.4	103
191	Color-tuning mechanism of firefly investigated by multi-configurational perturbation method. *Journal of the American Chemical Society*, **2010**, 132, 706-12	16.4	100
190	Chemiluminescence of 1,2-dioxetane. Reaction mechanism uncovered. *Journal of Physical Chemistry A*, **2007**, 111, 8013-9	2.8	95
189	The chemistry of bioluminescence: an analysis of chemical functionalities. *ChemPhysChem*, **2011**, 12, 3064-76	3.2	93
188	Theoretical study of the chemiluminescent decomposition of dioxetanone. *Journal of the American Chemical Society*, **2009**, 131, 6181-8	16.4	84
187	New General Tools for Constrained Geometry Optimizations. *Journal of Chemical Theory and Computation*, **2005**, 1, 1029-37	6.4	81
186	Ab Initio Study of the Bergman Reaction: The Autoaromatization of Hex-3-ene-1,5-diyne. *Journal of the American Chemical Society*, **1994**, 116, 4963-4969	16.4	78

185	Mapping the Excited State Potential Energy Surface of a Retinal Chromophore Model with Multireference and Equation-of-Motion Coupled-Cluster Methods. *Journal of Chemical Theory and Computation*, **2013**, 9, 4495-506	6.4	76
184	A theoretical study of the diffuseness of the V(1B1u) state of planar ethylene. *International Journal of Quantum Chemistry*, **1989**, 35, 813-825	2.1	76
183	Analytical State-Average Complete-Active-Space Self-Consistent Field Nonadiabatic Coupling Vectors: Implementation with Density-Fitted Two-Electron Integrals and Application to Conical Intersections. *Journal of Chemical Theory and Computation*, **2016**, 12, 3636-53	6.4	75
182	Agostic interaction in the methylidene metal dihydride complexes H2MCH2 (M=Y, Zr, Nb, Mo, Ru, Th, or U). *Journal of Physical Chemistry A*, **2007**, 111, 6420-4	2.8	75
181	Linear scaling multireference singles and doubles configuration interaction. *Journal of Chemical Physics*, **2008**, 128, 224106	3.9	74
180	Utilizing high performance computing for chemistry: parallel computational chemistry. *Physical Chemistry Chemical Physics*, **2010**, 12, 6896-920	3.6	73
179	Calibration of Cholesky Auxiliary Basis Sets for Multiconfigurational Perturbation Theory Calculations of Excitation Energies. *Journal of Chemical Theory and Computation*, **2010**, 6, 747-54	6.4	73
178	Integral-direct electron correlation methods. *Molecular Physics*, **1999**, 96, 719-733	1.7	73
177	Theoretical study of the electronic ground state of iron(II) porphine. II. *Journal of Chemical Physics*, **1999**, 111, 3837-3845	3.9	72
176	Benzophenone Ultrafast Triplet Population: Revisiting the Kinetic Model by Surface-Hopping Dynamics. *Journal of Physical Chemistry Letters*, **2016**, 7, 622-6	6.4	71
175	Systematic Theoretical Investigation on the Light Emitter of Firefly. *Journal of Chemical Theory and Computation*, **2011**, 7, 798-803	6.4	71
174	Simple N[triple bond]UF3 and P[triple bond]UF3 molecules with triple bonds to uranium. *Angewandte Chemie - International Edition*, **2008**, 47, 5366-70	16.4	71
173	Dissociation reaction of N8 azapentalene to 4N2: A theoretical study. *International Journal of Quantum Chemistry*, **2000**, 77, 311-315	2.1	67
172	On the use of a Hessian model function in molecular geometry optimizations. *Chemical Physics Letters*, **1995**, 241, 423-428	2.5	67
171	The Matter Simulation (R)evolution. *ACS Central Science*, **2018**, 4, 144-152	16.8	66
170	Symmetry breaking in O+4: an application of the Brueckner coupled-cluster method. *Chemical Physics Letters*, **1994**, 223, 207-214	2.5	66
169	Benzyne Thermochemistry: A Benchmark ab Initio Study. *Journal of Physical Chemistry A*, **1999**, 103, 9913-9920	2.8	64
168	MOLCAS 8: new capabilities for multiconfigurational quantum chemical calculations across solid state. *Journal of Computational Chemistry*, **2015**, 36, 506-20	3.8	61
167	MOLCAS: a program package for computational chemistry. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2013**, 3, 143-149	7.9	61

167	Cholesky Decomposition Techniques in Electronic Structure Theory. *Challenges and Advances in Computational Chemistry and Physics*, **2011**, 301-343	0.7	61
166	Analytic high-order Douglas-Kroll-Hess electric field gradients. *Journal of Chemical Physics*, **2007**, 127, 074105	3.9	60
165	Quantum chemistry on parallel computer architectures: coupled-cluster theory applied to the bending potential of fulminic acid. *Chemical Physics Letters*, **1992**, 194, 84-94	2.5	60
164	Analytical gradients of a state average MCSCF state and a state average diagnostic. *Molecular Physics*, **2001**, 99, 103-114	1.7	59
163	**2016**,		59
162	How machine learning can assist the interpretation of molecular dynamics simulations and conceptual understanding of chemistry. *Chemical Science*, **2019**, 10, 2298-2307	9.4	58
161	Analytic derivatives for the Cholesky representation of the two-electron integrals. *Journal of Chemical Physics*, **2008**, 129, 034106	3.9	57
160	Relativistic and correlated calculations on the ground and excited states of ThO. *Journal of Chemical Physics*, **2003**, 119, 798-805	3.9	57
159	Ab initio investigation on the chemical origin of the firefly bioluminescence. *Journal of Photochemistry and Photobiology A: Chemistry*, **2008**, 194, 261-267	4.7	56
158	Molecular integrals by numerical quadrature. I. Radial integration. *Theoretical Chemistry Accounts*, **2001**, 106, 178-187	1.9	56
157	Attractive electron-electron interactions within robust local fitting approximations. *Journal of Computational Chemistry*, **2013**, 34, 1486-96	3.5	52
156	Correlation potentials for a multiconfigurational-based density functional theory with exact exchange. *Theoretical Chemistry Accounts*, **2004**, 112, 84-94	1.9	52
155	Ab Initio Density Fitting: Accuracy Assessment of Auxiliary Basis Sets from Cholesky Decompositions. *Journal of Chemical Theory and Computation*, **2009**, 5, 1545-53	6.4	51
154	Unique QM/MM potential energy surface exploration using microiterations. *International Journal of Quantum Chemistry*, **2011**, 111, 3339-3346	2.1	50
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152	Orbital entanglement and CASSCF analysis of the Ru-NO bond in a Ruthenium nitrosyl complex. *Physical Chemistry Chemical Physics*, **2015**, 17, 14383-92	3.6	49
151	Accurate calculations of geometries and singlet-triplet energy differences for active-site models of [NiFe] hydrogenase. *Physical Chemistry Chemical Physics*, **2014**, 16, 7927-38	3.6	48
150	The reduced multiplication scheme of the Rys-Gauss quadrature for 1st order integral derivatives. *Theoretica Chimica Acta*, **1993**, 85, 423-440		48

149	Metal-free photochemical silylations and transfer hydrogenations of benzenoid hydrocarbons and graphene. *Nature Communications*, **2016**, 7, 12962	17.4	47
148	A CAS SCF CI study of the hydrogen migration potential in protonated acetylene, C2H3+. *Chemical Physics Letters*, **1987**, 139, 407-416	2.5	47
147	Unraveling factors leading to efficient norbornadiene–quadricyclane molecular solar-thermal energy storage systems. *Journal of Materials Chemistry A*, **2017**, 5, 12369-12378	13	46
146	Electronic structure of the two isomers of the anionic form of p-coumaric acid chromophore. *Journal of Chemical Physics*, **2011**, 134, 034310	3.9	46
145	A CASSCF/CASPT2 approach to the decomposition of thiazole-substituted dioxetanone: Substitution effects and charge-transfer induced electron excitation. *Chemical Physics Letters*, **2009**, 484, 69-75	2.5	46
144	Using on-top pair density for construction of correlation functionals for multideterminant wave functions. *Molecular Physics*, **2004**, 102, 2207-2216	1.7	46
143	Are the bio- and chemiluminescence states of the firefly oxyluciferin the same as the fluorescence state?. *Photochemistry and Photobiology*, **2013**, 89, 319-25	3.6	45
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140	Multi-electron integrals. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 290-303	7.9	44
139	The energy separation between the classical and nonclassical isomers of protonated acetylene. An extensive study in one- and n-particle space. *Journal of Chemical Physics*, **1991**, 94, 8008-8014	3.9	44
138	Essential on the Photophysics and Photochemistry of the Indole Chromophore by Using a Totally Unconstrained Theoretical Approach. *Journal of Chemical Theory and Computation*, **2011**, 7, 4088-96	6.4	43
137	Analytical gradients of complete active space self-consistent field energies using Cholesky decomposition: geometry optimization and spin-state energetics of a ruthenium nitrosyl complex. *Journal of Chemical Physics*, **2014**, 140, 174103	3.9	42
136	The Douglas–Kroll–Hess electron density at an atomic nucleus. *Chemical Physics Letters*, **2008**, 465, 157-164	2.5	42
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133	Embedding Fragment ab Initio Model Potentials in CASSCF/CASPT2 Calculations of Doped Solids: Implementation and Applications. *Journal of Chemical Theory and Computation*, **2008**, 4, 586-94	6.4	41
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131	The fraternal twins of quartet O+4. *Journal of Chemical Physics*, **1994**, 100, 224-237	3.9	39
130	Proton/Hydrogen Transfer Mechanisms in the Guanine-Cytosine Base Pair: Photostability and Tautomerism. *Journal of Chemical Theory and Computation*, **2013**, 9, 481-96	6.4	38
129	Ab initio model potential embedded-cluster study of the ground and lowest excited states of Cr3+ defects in the elpasolites Cs2NaYCl6 and Cs2NaYBr6. *Journal of Chemical Physics*, **1998**, 108, 2005-2014	3.9	37
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126	Automatic Differentiation in Quantum Chemistry with Applications to Fully Variational Hartree-Fock. *ACS Central Science*, **2018**, 4, 559-566	16.8	35
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122	Revisiting the Nonadiabatic Process in 1,2-Dioxetane. *Journal of Chemical Theory and Computation*, **2013**, 9, 5404-11	6.4	32
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119	The ammonia dimer equilibrium dissociation energy: convergence to the basis set limit at the correlated level. *Molecular Physics*, **2002**, 100, 3389-3399	1.7	30
118	Parallelization of a multiconfigurational perturbation theory. *Journal of Computational Chemistry*, **2013**, 34, 1937-48	3.5	29
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114	Force-constant weighted redundant coordinates in molecular geometry optimizations. *Chemical Physics Letters*, **1999**, 303, 567-575	2.5	28

113	Direct self-consistent reaction field with Pauli repulsion: solvation effects on methylene peroxide. *Chemical Physics Letters*, **1996**, 251, 141-149	2.5	28
112	Automation of Active Space Selection for Multireference Methods via Machine Learning on Chemical Bond Dissociation. *Journal of Chemical Theory and Computation*, **2020**, 16, 2389-2399	6.4	27
111	Analytic Gradients for Complete Active Space Pair-Density Functional Theory. *Journal of Chemical Theory and Computation*, **2018**, 14, 126-138	6.4	27
110	Analytical gradients of the state-average complete active space self-consistent field method with density fitting. *Journal of Chemical Physics*, **2015**, 143, 044110	3.9	27
109	Basis set representation of the electron density at an atomic nucleus. *Journal of Chemical Physics*, **2010**, 133, 144111	3.9	27
108	A direct implementation of the second-order derivatives of multiconfigurational SCF energies and an analysis of the preconditioning in the associated response equation. *Molecular Physics*, **1999**, 96, 617-628	1.7	27
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94	Theoretical studies of isomers of C3H2 using a multiconfigurational approach. *Theoretical Chemistry Accounts*, **2000**, 105, 15-30	1.9	20
93	Theoretical study of the dark photochemistry of 1,3-butadiene via the chemiexcitation of Dewar dioxetane. *Physical Chemistry Chemical Physics*, **2015**, 17, 18653-64	3.6	19
92	Dynamical Insights into the Decomposition of 1,2-Dioxetane. *Journal of Chemical Theory and Computation*, **2017**, 13, 2448-2457	6.4	18
91	Symmetry of three-center, four-electron bonds. *Chemical Science*, **2020**, 11, 7979-7990	9.4	18
90	Analytical gradients of the second-order M□llerPlesset energy using Cholesky decompositions. *International Journal of Quantum Chemistry*, **2014**, 114, 321-327	2.1	18
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87	Different bases for different correlation effects: multireference M□llerPlesset perturbation theory in the extended basis function space. *Chemical Physics Letters*, **1999**, 300, 303-311	2.5	16
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84	An integral direct, distributed-data, parallel MP2 algorithm. *Theoretica Chimica Acta*, **1997**, 95, 13-34		14
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72	Integral-direct electron correlation methods		11
71	Semiclassical Molecular Dynamics for Spectroscopic Calculations **2020**, 595-628		11
70	Dynamically weighted multireference perturbation theory: Combining the advantages of multi-state and state-averaged methods. *Journal of Chemical Physics*, **2019**, 150, 144107	3.9	10
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