Roland H Lindh

List of Publications by Year in Descending Order

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	Restricted-Variance Constrained, Reaction Path, and Transition State Molecular Optimizations Using Gradient-Enhanced Kriging. *Journal of Chemical Theory and Computation*, **2021**, 17, 571-582	6.4	8
219	,-Chelated Gold(III) Complexes: Structure and Reactivity. *Inorganic Chemistry*, **2021**, 60, 2847-2855	5.1	6
218	Analytic gradients for multiconfiguration pair-density functional theory with density fitting: Development and application to geometry optimization in the ground and excited states. *Journal of Chemical Physics*, **2021**, 154, 074108	3.9	2
217	On the role of symmetry in XDW-CASPT2. *Journal of Chemical Physics*, **2021**, 154, 034102	3.9	3
216	Halogen Bond of Halonium Ions: Benchmarking DFT Methods for the Description of NMR Chemical Shifts. *Journal of Chemical Theory and Computation*, **2020**, 16, 7690-7701	6.4	4
215	Restricted-Variance Molecular Geometry Optimization Based on Gradient-Enhanced Kriging. *Journal of Chemical Theory and Computation*, **2020**, 16, 3989-4001	6.4	13
214	Impact of Excited-State Antiaromaticity Relief in a Fundamental Benzene Photoreaction Leading to Substituted Bicyclo[3.1.0]hexenes. *Journal of the American Chemical Society*, **2020**, 142, 10942-10954	16.4	12
213	Modern quantum chemistry with [Open]Molcas. *Journal of Chemical Physics*, **2020**, 152, 214117	3.9	106
212	Simulations of valence excited states in coordination complexes reached through hard X-ray scattering. *Physical Chemistry Chemical Physics*, **2020**, 22, 8325-8335	3.6	5
211	Symmetry of three-center, four-electron bonds. *Chemical Science*, **2020**, 11, 7979-7990	9.4	18
210	Machine learning for analysing ab initio molecular dynamics simulations. *Journal of Physics: Conference Series*, **2020**, 1412, 042003	0.3	1
209	Extended Dynamically Weighted CASPT2: The Best of Two Worlds. *Journal of Chemical Theory and Computation*, **2020**, 16, 1555-1567	6.4	16
208	Non-radiative decay and fragmentation in water molecules after 1a 4a excitation and core ionization studied by electron-energy-resolved electron-ion coincidence spectroscopy. *Journal of Chemical Physics*, **2020**, 152, 074302	3.9	0
207	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
206	Quantifying similarity for spectra with a large number of overlapping transitions: Examples from soft X-ray spectroscopy. *Chemical Physics*, **2020**, 535, 110786	2.3	5
205	Equation-of-Motion Coupled-Cluster Models **2020**, 77-108		2
204	Multi-Reference Configuration Interaction **2020**, 277-297		1

203	Unravelling the mechanism of pH-regulation in dinoflagellate luciferase. *International Journal of Biological Macromolecules*, **2020**, 164, 2671-2680	7.9	
202	Path-Integral Approaches to Non-Adiabatic Dynamics **2020**, 629-653		3
201	Multi-Configurational Density Functional Theory: Progress and Challenges **2020**, 47-75		1
200	Bohmian Approaches to Non-Adiabatic Molecular Dynamics **2020**, 563-594		0
199	Time-Dependent Density Functional Theory **2020**, 13-46		6
198	Exact Quantum Dynamics (Wave Packets) in Reduced Dimensionality **2020**, 355-381		4
197	Full and Ab Initio Multiple Spawning **2020**, 435-467		3
196	Surface Hopping Molecular Dynamics **2020**, 499-530		4
195	Exact Factorization of the Electron Nuclear Wave Function: Theory and Applications **2020**, 531-562		6
194	Exact semi-classical light-matter interaction operator applied to two-photon processes with strong relativistic effects. *Journal of Chemical Physics*, **2020**, 153, 024114	3.9	1
193	Motivation and Basic Concepts **2020**, 1-12		
192	Multi-Configuration Time-Dependent Hartree Methods: From Quantum to Semiclassical and Quantum-Classical **2020**, 383-411		3
191	Gaussian Wave Packets and the DD-vMCG Approach **2020**, 413-433		1
190	Semiclassical Molecular Dynamics for Spectroscopic Calculations **2020**, 595-628		11
189	Multi-Configurational Reference Perturbation Theory with a CASSCF Reference Function **2020**, 299-353		3
188	The Algebraic-Diagrammatic Construction Scheme for the Polarization Propagator **2020**, 109-131		2
187	Foundation of Multi-Configurational Quantum Chemistry **2020**, 133-203		3
186	The Density Matrix Renormalization Group for Strong Correlation in Ground and Excited States **2020**, 205-245		7

185	Excited-State Calculations with Quantum Monte Carlo **2020**, 247-275		6
184	OpenMolcas: From Source Code to Insight. *Journal of Chemical Theory and Computation*, **2019**, 15, 5925-5964	5.4	310
183	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
182	Molecular Basis of the Chemiluminescence Mechanism of Luminol. *Chemistry - A European Journal*, **2019**, 25, 5202-5213	4.8	24
181	Spectroscopy of linear and circular polarized light with the exact semiclassical light–matter interaction. *Annual Reports in Computational Chemistry*, **2019**, 15, 39-76	1.8	3
180	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
179	Implementation of a semiclassical light-matter interaction using the Gauss-Hermite quadrature: A simple alternative to the multipole expansion. *Physical Review A*, **2019**, 99,	2.6	9
178	Fingerprinting Electronic Structure of Heme Iron by Ab Initio Modeling of Metal L-Edge X-ray Absorption Spectra. *Journal of Chemical Theory and Computation*, **2019**, 15, 477-489	6.4	14
177	Chemi- and Bioluminescence of Cyclic Peroxides. *Chemical Reviews*, **2018**, 118, 6927-6974	68.1	172
176	QM/MM Study of the Formation of the Dioxetanone Ring in Fireflies through a Superoxide Ion. *Journal of Physical Chemistry B*, **2018**, 122, 5173-5182	3.4	10
175	The Matter Simulation (R)evolution. *ACS Central Science*, **2018**, 4, 144-152	16.8	66
174	Analytic Gradients for Complete Active Space Pair-Density Functional Theory. *Journal of Chemical Theory and Computation*, **2018**, 14, 126-138	6.4	27
173	Automatic Differentiation in Quantum Chemistry with Applications to Fully Variational Hartree-Fock. *ACS Central Science*, **2018**, 4, 559-566	16.8	35
172	Uncontracted basis sets for ab initio calculations of muonic atoms and molecules. *International Journal of Quantum Chemistry*, **2018**, 118, e25755	2.1	3
171	Inner projection techniques for the low-cost handling of two-electron integrals in quantum chemistry. *Molecular Physics*, **2017**, 115, 2052-2064	1.7	8
170	Triplet versus singlet chemiexcitation mechanism in dioxetanone: a CASSCF/CASPT2 study. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	7
169	Dynamical Insights into the Decomposition of 1,2-Dioxetane. *Journal of Chemical Theory and Computation*, **2017**, 13, 2448-2457	6.4	18
168	Gauge origin independence in finite basis sets and perturbation theory. *Chemical Physics Letters*, **2017**, 683, 536-542	2.5	9

167	Unraveling factors leading to efficient norbornadiene□quadricyclane molecular solar-thermal energy storage systems. *Journal of Materials Chemistry A*, **2017**, 5, 12369-12378	13	46
166	Influence of the choice of projection manifolds in the CASPT2 implementation. *Molecular Physics*, **2017**, 115, 2077-2085	1.7	3
165	Mechanism of activated chemiluminescence of cyclic peroxides: 1,2-dioxetanes and 1,2-dioxetanones. *Physical Chemistry Chemical Physics*, **2017**, 19, 3955-3962	3.6	25
164	A celebration of the Swedish school. *Molecular Physics*, **2017**, 115, 1993-1994	1.7	1
163	How Do Methyl Groups Enhance the Triplet Chemiexcitation Yield of Dioxetane?. *Journal of Physical Chemistry Letters*, **2017**, 8, 3790-3794	6.4	16
162	Applications to metal K pre-edges of transition metal dimers illustrate the approximate origin independence for the intensities in the length representation. *Molecular Physics*, **2017**, 115, 174-189	1.7	21
161	CASPT2/CASSCF Applications **2016**, 157-219		2
160	Relativistic Effects **2016**, 59-67		
159	Basis Sets **2016**, 69-84		
158	Molecular and Electronic Structure of Re2Br4(PMe3)4. *Inorganic Chemistry*, **2016**, 55, 7111-6	5.1	1
157	Metal-free photochemical silylations and transfer hydrogenations of benzenoid hydrocarbons and graphene. *Nature Communications*, **2016**, 7, 12962	17.4	47
156	Analysis of a Compound Class with Triplet States Stabilized by Potentially Baird Aromatic [10]Annulenyl Dicationic Rings. *Chemistry - A European Journal*, **2016**, 22, 2793-800	4.8	25
155	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
154	Benzophenone Ultrafast Triplet Population: Revisiting the Kinetic Model by Surface-Hopping Dynamics. *Journal of Physical Chemistry Letters*, **2016**, 7, 622-6	6.4	71
153	Advances in computational photochemistry and chemiluminescence of biological and nanotechnological molecules. *Photochemistry*, **2016**, 16-60	1.8	2
152	Large-scale calculations of gas phase thermochemistry: Enthalpy of formation, standard entropy, and heat capacity. *Journal of Chemical Physics*, **2016**, 145, 114305	3.9	42
151	Molcas 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. *Journal of Computational Chemistry*, **2016**, 37, 506-41	3.5	1047
150	**2016**,		59

149	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
148	What Is the Price of Open-Source Software?. *Journal of Physical Chemistry Letters*, **2015**, 6, 2751-4	6.4	8
147	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
146	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
145	Influence of Alkoxy Groups on the Photoinduced Dynamics of Organic Molecules Exemplified on Alkyl Vinyl Ethers. *Journal of Physical Chemistry A*, **2015**, 119, 11105-12	2.8	9
144	Constrained numerical gradients and composite gradients: Practical tools for geometry optimization and potential energy surface navigation. *Journal of Computational Chemistry*, **2015**, 36, 1698-708	3.5	4
143	A surface hopping algorithm for nonadiabatic minimum energy path calculations. *Journal of Computational Chemistry*, **2015**, 36, 312-20	3.5	6
142	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
141	Analytical gradients of the second-order M□llerPlesset energy using Cholesky decompositions. *International Journal of Quantum Chemistry*, **2014**, 114, 321-327	2.1	18
140	Hybrid QM/MM simulations of the obelin bioluminescence and fluorescence reveal an unexpected light emitter. *Journal of Physical Chemistry B*, **2014**, 118, 2896-903	3.4	28
139	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
138	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
137	Chapter 2:Recent method developments and applications in computational photochemistry, chemiluminescene and bioluminescence. *Photochemistry*, **2014**, 11-42	1.8	2
136	S0 -iS3 transition in recombination products of photodissociated dihalomethanes. *Molecular Physics* , **2014**, 112, 575-582	1.7	1
135	A theoretical analysis of the intrinsic light-harvesting properties of xanthopterin. *Computational and Theoretical Chemistry*, **2014**, 1040-1041, 230-236	2	1
134	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
133	Revisiting the Nonadiabatic Process in 1,2-Dioxetane. *Journal of Chemical Theory and Computation*, **2013**, 9, 5404-11	6.4	32
132	Analytical Gradients of Hartree-Fock Exchange with Density Fitting Approximations. *Journal of Chemical Theory and Computation*, **2013**, 9, 204-12	6.4	24

131	MOLCAS□ software for multiconfigurational quantum chemistry calculations. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2013**, 3, 143-149	7.9	61
130	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
129	Attractive electron-electron interactions within robust local fitting approximations. *Journal of Computational Chemistry*, **2013**, 34, 1486-96	3.5	52
128	Ab initio and DFT analysis of the low-lying electronic states of metal dihalides: quantum chemical calculations on the neutral BrMCl (M = Cu, Ag, Au). *Physical Chemistry Chemical Physics*, **2013**, 15, 10151-7	3.6	
127	Parallelization of a multiconfigurational perturbation theory. *Journal of Computational Chemistry*, **2013**, 34, 1937-48	3.5	29
126	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
125	Communication: theoretical prediction of the structure and spectroscopic properties of the X and states of hydroxymethyl peroxy (HOCH2OO) radical. *Journal of Chemical Physics*, **2013**, 138, 021105	3.9	4
124	The Bergman cyclizations of the enediyne and its N-substituted analogs using multiconfigurational second-order perturbation theory. *Journal of Computational Chemistry*, **2012**, 33, 537-49	3.5	13
123	Can the Closed-Shell DFT Methods Describe the Thermolysis of 1,2-Dioxetanone?. *Journal of Chemical Theory and Computation*, **2012**, 8, 4359-63	6.4	26
122	Chemiluminescence of Coelenterazine and Fluorescence of Coelenteramide: A Systematic Theoretical Study. *Journal of Chemical Theory and Computation*, **2012**, 8, 2796-807	6.4	39
121	Novel insights into cyclooxygenases, linoleate diol synthases, and lipoxygenases from deuterium kinetic isotope effects and oxidation of substrate analogs. *Biochimica Et Biophysica Acta - Molecular and Cell Biology of Lipids*, **2012**, 1821, 1508-17	5	11
120	Variational calculations for the hydrogen-antihydrogen system with a mass-scaled Born-Oppenheimer potential. *Open Physics*, **2012**, 10,	1.3	4
119	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
118	Photostability Mechanisms in Human B-Crystallin: Role of the Tyrosine Corner Unveiled by Quantum Mechanics and Hybrid Quantum Mechanics/Molecular Mechanics Methodologies. *Journal of Chemical Theory and Computation*, **2012**, 8, 1351-9	6.4	4
117	On the photophysics and photochemistry of the water dimer. *Journal of Chemical Physics*, **2012**, 137, 244309	3.9	22
116	Multi-electron integrals. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 290-303	7.9	44
115	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
114	Coupled Cluster and M□ller-Plesset Perturbation Theory Calculations of Noncovalent Intermolecular Interactions using Density Fitting with Auxiliary Basis Sets from Cholesky Decompositions. *Journal of Chemical Theory and Computation*, **2012**, 8, 1921-8	6.4	32

113	Comment on "Density functional theory study of 1,2-dioxetanone decomposition in condensed phase". *Journal of Computational Chemistry*, **2012**, 33, 2124-6; author reply 2127-30	3.5	11
112	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
111	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
110	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
109	Systematic Theoretical Investigation on the Light Emitter of Firefly. *Journal of Chemical Theory and Computation*, **2011**, 7, 798-803	6.4	71
108	Chemiluminescence and Fluorescence States of a Small Model for Coelenteramide and Cypridina Oxyluciferin: A CASSCF/CASPT2 Study. *Journal of Chemical Theory and Computation*, **2011**, 7, 4060-9	6.4	45
107	Multireference theoretical studies on the solvent effect of firefly multicolor bioluminescence. *International Journal of Quantum Chemistry*, **2011**, 111, 3371-3377	2.1	12
106	Unique QM/MM potential energy surface exploration using microiterations. *International Journal of Quantum Chemistry*, **2011**, 111, 3339-3346	2.1	50
105	The chemistry of bioluminescence: an analysis of chemical functionalities. *ChemPhysChem*, **2011**, 12, 3064-76	3.2	93
104	Cholesky Decomposition Techniques in Electronic Structure Theory. *Challenges and Advances in Computational Chemistry and Physics*, **2011**, 301-343	0.7	61
103	Utilizing high performance computing for chemistry: parallel computational chemistry. *Physical Chemistry Chemical Physics*, **2010**, 12, 6896-920	3.6	73
102	Color-tuning mechanism of firefly investigated by multi-configurational perturbation method. *Journal of the American Chemical Society*, **2010**, 132, 706-12	16.4	100
101	Basis set representation of the electron density at an atomic nucleus. *Journal of Chemical Physics*, **2010**, 133, 144111	3.9	27
100	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
99	MOLCAS 7: the next generation. *Journal of Computational Chemistry*, **2010**, 31, 224-47	3.5	1425
98	A NEMO potential that includes the dipole-quadrupole and quadrupole-quadrupole polarizability. *Journal of Computational Chemistry*, **2010**, 31, 1583-91	3.5	45
97	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
96	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

95	Density fitting with auxiliary basis sets from Cholesky decompositions. *Theoretical Chemistry Accounts*, **2009**, 124, 1-10	1.9	123
94	Role of electronic curve crossing of benzene S1 state in the photodissociation of aryl halides, effect of fluorination: RASSI-SO MS-CASPT2 study. *International Journal of Quantum Chemistry*, **2009**, 109, 1962-1974	2.1	7
93	Theoretical study of the chemiluminescent decomposition of dioxetanone. *Journal of the American Chemical Society*, **2009**, 131, 6181-8	16.4	84
92	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
91	Location of Two Seams in the Proximity of the C2v Minimum Energy Path of Formaldehyde. *Journal of Chemical Theory and Computation*, **2009**, 5, 186-91	6.4	6
90	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
89	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
88	Nuclear quadrupole moment of 119Sn. *Journal of Physical Chemistry A*, **2008**, 112, 1666-72	2.8	36
87	Analytic derivatives for the Cholesky representation of the two-electron integrals. *Journal of Chemical Physics*, **2008**, 129, 034106	3.9	57
86	Linear scaling multireference singles and doubles configuration interaction. *Journal of Chemical Physics*, **2008**, 128, 224106	3.9	74
85	A combined theoretical and experimental study of simple terminal group 6 nitride and phosphide N[triple bond]MX3 and P[triple bond]MX3 molecules. *Journal of Physical Chemistry A*, **2008**, 112, 8030-7	2.8	26
84	Accurate ab initio density fitting for multiconfigurational self-consistent field methods. *Journal of Chemical Physics*, **2008**, 129, 024113	3.9	145
83	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
82	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
81	The Douglas Kroll Hess electron density at an atomic nucleus. *Chemical Physics Letters*, **2008**, 465, 157-164	2.5	42
80	Chemiluminescence of 1,2-dioxetane. Reaction mechanism uncovered. *Journal of Physical Chemistry A*, **2007**, 111, 8013-9	2.8	95
79	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
78	Accuracy of distributed multipoles and polarizabilities: comparison between the LoProp and MpProp models. *Journal of Computational Chemistry*, **2007**, 28, 1083-90	3.5	29

77	Spin-orbit ab initio investigation of the ultraviolet photolysis of diiodomethane. *ChemPhysChem*, **2007**, 8, 890-8	3.2	21
76	The charge capacity of the chemical bond. *Chemical Physics Letters*, **2007**, 436, 297-301	2.5	6
75	Ab initio DFT study of ZE isomerization pathways of N-benzylideneaniline. *Theoretical Chemistry Accounts*, **2007**, 118, 271-279	1.9	26
74	Analytic high-order Douglas-Kroll-Hess electric field gradients. *Journal of Chemical Physics*, **2007**, 127, 074105	3.9	60
73	A combined experimental and theoretical study of uranium polyhydrides with new evidence for the large complex UH4(H2)6. *Journal of Physical Chemistry A*, **2007**, 111, 6383-7	2.8	34
72	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
71	Unbiased auxiliary basis sets for accurate two-electron integral approximations. *Journal of Chemical Physics*, **2007**, 127, 114107	3.9	228
70	The prediction of the nuclear quadrupole splitting of 119Sn Mössbauer spectroscopy data by scalar relativistic DFT calculations. *Chemistry - A European Journal*, **2006**, 12, 5116-21	4.8	10
69	Spin-orbit ab initio investigation of the photolysis of bromoiodomethane. *ChemPhysChem*, **2006**, 7, 955-63	3.2	23
68	New relativistic ANO basis sets for transition metal atoms. *Journal of Physical Chemistry A*, **2005**, 109, 6575-9	2.8	799
67	New relativistic ANO basis sets for actinide atoms. *Chemical Physics Letters*, **2005**, 409, 295-299	2.5	220
66	New General Tools for Constrained Geometry Optimizations. *Journal of Chemical Theory and Computation*, **2005**, 1, 1029-37	6.4	81
65	Computation of conical intersections by using perturbation techniques. *Journal of Chemical Physics*, **2005**, 122, 104107	3.9	107
64	Local properties of quantum chemical systems: the LoProp approach. *Journal of Chemical Physics*, **2004**, 121, 4494-500	3.9	282
63	Spin-orbit ab initio study of alkyl halide dissociation via electronic curve crossing. *Journal of Chemical Physics*, **2004**, 121, 5761-6	3.9	42
62	Correlation potentials for a multiconfigurational-based density functional theory with exact exchange. *Theoretical Chemistry Accounts*, **2004**, 112, 84-94	1.9	52
61	2MOLCAS as a development platform for quantum chemistry software. *International Journal of Quantum Chemistry*, **2004**, 100, 626-635	2.1	293
60	Using on-top pair density for construction of correlation functionals for multideterminant wave functions. *Molecular Physics*, **2004**, 102, 2207-2216	1.7	46

59	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
58	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
57	Semidirect parallel self-consistent field: the load balancing problem in the input/output intensive self-consistent field iterations. *Theoretical Chemistry Accounts*, **2003**, 110, 156-164	1.9	6
56	Björn's top ten. *Theoretical Chemistry Accounts*, **2003**, 110, 115-117	1.9	1
55	Photodissociation of bromobenzene in solution. *Chemical Physics Letters*, **2003**, 367, 759-766	2.5	32
54	MOLCAS: a program package for computational chemistry. *Computational Materials Science*, **2003**, 28, 222-239	3.2	1617
53	Relativistic and correlated calculations on the ground and excited states of ThO. *Journal of Chemical Physics*, **2003**, 119, 798-805	3.9	57
52	A theoretical study of the 21Ag <- 11Ag two-photon transition and its vibronic band in trans-stilbene. *Molecular Physics*, **2002**, 100, 1791-1796	1.7	5
51	Analysis of the Relative Stability of cis-Urocanic Acid in Condensed Phase. The Use of Langevin Dipoles. *Journal of Physical Chemistry B*, **2002**, 106, 7115-7120	3.4	4
50	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
49	Molecular integrals by numerical quadrature. I. Radial integration. *Theoretical Chemistry Accounts*, **2001**, 106, 178-187	1.9	56
48	Analytical gradients of a state average MCSCF state and a state average diagnostic. *Molecular Physics*, **2001**, 99, 103-114	1.7	59
47	Dissociation reaction of N8 azapentalene to 4N2: A theoretical study. *International Journal of Quantum Chemistry*, **2000**, 77, 311-315	2.1	67
46	Theoretical studies of isomers of C3H2 using a multiconfigurational approach. *Theoretical Chemistry Accounts*, **2000**, 105, 15-30	1.9	20
45	Integral-direct electron correlation methods. *Molecular Physics*, **1999**, 96, 719-733	1.7	73
44	Different bases for different correlation effects: multireference Møller–Plesset perturbation theory in the extended basis function space. *Chemical Physics Letters*, **1999**, 300, 303-311	2.5	16
43	Force-constant weighted redundant coordinates in molecular geometry optimizations. *Chemical Physics Letters*, **1999**, 303, 567-575	2.5	28
42	Theoretical study of the electronic ground state of iron(II) porphine. II. *Journal of Chemical Physics*, **1999**, 111, 3837-3845	3.9	72

41	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
40	Benzyne Thermochemistry: A Benchmark ab Initio Study. *Journal of Physical Chemistry A*, **1999**, 103, 9913-9920	2.8	64
39	On the Thermodynamic Stability of ArO4. *Journal of Physical Chemistry A*, **1999**, 103, 8295-8302	2.8	13
38	Tetramethylene: A CASPT2 study. *Chemical Physics Letters*, **1998**, 289, 442-450	2.5	34
37	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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