Thomas B Pedersen

List of Publications by Year
in descending order

79 papers	8,913 citations	71097 41 h-index	74160 75 g-index
79 all docs	79 docs citations	79 times ranked	6016 citing authors

#	Article	IF	Citations
1	MOLCAS 7: The Next Generation. Journal of Computational Chemistry, 2010, 31, 224-247.	3.3	1,485
2	<scp>Molcas</scp> 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. Journal of Computational Chemistry, 2016, 37, 506-541.	3.3	1,317
3	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	14.6	1,166
4	Reduced scaling in electronic structure calculations using Cholesky decompositions. Journal of Chemical Physics, 2003, 118, 9481-9484.	3.0	386
5	Cholesky Decomposition-Based Multiconfiguration Second-Order Perturbation Theory (CD-CASPT2): Application to the Spin-State Energetics of Co^{III}(diiminato)(NPh). Journal of Chemical Theory and Computation, 2008, 4, 694-702.	5.3	336
6	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.	3.0	285
7	Modern quantum chemistry with [Open]Molcas. Journal of Chemical Physics, 2020, 152, 214117.	3.0	281
8	Unbiased auxiliary basis sets for accurate two-electron integral approximations. Journal of Chemical Physics, 2007, 127, 114107.	3.0	279
9	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.	3.0	185
10	Accurate ab initio density fitting for multiconfigurational self-consistent field methods. Journal of Chemical Physics, 2008, 129, 024113.	3.0	161
11	Origin invariant calculation of optical rotation without recourse to London orbitals. Chemical Physics Letters, 2004, 393, 319-326.	2.6	156
12	Density fitting with auxiliary basis sets from Cholesky decompositions. Theoretical Chemistry Accounts, 2009, 124, 1-10.	1.4	142
13	Fast noniterative orbital localization for large molecules. Journal of Chemical Physics, 2006, 125, 174101.	3.0	138
14	Coupled cluster response functions revisited. Journal of Chemical Physics, 1997, 106, 8059-8072.	3.0	120
15	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, 3636-3653.	5.3	112
16	Polarizability and optical rotation calculated from the approximate coupled cluster singles and doubles CC2 linear response theory using Cholesky decompositions. Journal of Chemical Physics, 2004, 120, 8887-8897.	3.0	107
17	Gauge invariant coupled cluster response theory. Journal of Chemical Physics, 1999, 110, 8318-8327.	3.0	96
18	Coupled cluster calculations of the optical rotation of S-propylene oxide in gas phase and solution. Chemical Physics Letters, 2005, 401, 385-392.	2.6	94

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19	The heliumâ€“, neonâ€“, and argonâ€“cyclopropane van der Waals complexes: Ab initio ground state intermolecular potential energy surfaces and intermolecular dynamics. Journal of Chemical Physics, 2001, 115, 8431-8439.	3.0	84
20	Gauge invariant coupled cluster response theory using optimized nonorthogonal orbitals. Journal of Chemical Physics, 2001, 114, 6983-6993.	3.0	82
21	Calibration of Cholesky Auxiliary Basis Sets for Multiconfigurational Perturbation Theory Calculations of Excitation Energies. Journal of Chemical Theory and Computation, 2010, 6, 747-754.	5.3	79
22	Coupled Cluster and Density Functional Theory Studies of the Vibrational Contribution to the Optical Rotation of (S)-Propylene Oxide. Journal of the American Chemical Society, 2006, 128, 976-982.	13.7	77
23	Coupled cluster response calculation of natural chiroptical spectra. Journal of Chemical Physics, 1999, 110, 2883-2892.	3.0	75
24	Cholesky Decomposition Techniques in Electronic Structure Theory. Challenges and Advances in Computational Chemistry and Physics, 2011, , 301-343.	0.6	71
25	Attractive electronâ€“electron interactions within robust local fitting approximations. Journal of Computational Chemistry, 2013, 34, 1486-1496.	3.3	67
26	MOLCASâ€”a software for multiconfigurational quantum chemistry calculations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 143-149.	14.6	66
27	Ab initio calculation and display of the rotary strength tensor in the random phase approximation. Method and model studies. Chemical Physics Letters, 1995, 246, 1-8.	2.6	64
28	Analytic derivatives for the Cholesky representation of the two-electron integrals. Journal of Chemical Physics, 2008, 129, 034106.	3.0	61
29	Orbital entanglement and CASSCF analysis of the Ruâ€“NO bond in a Ruthenium nitrosyl complex. Physical Chemistry Chemical Physics, 2015, 17, 14383-14392.	2.8	58
30	Ab Initio Density Fitting: Accuracy Assessment of Auxiliary Basis Sets from Cholesky Decompositions. Journal of Chemical Theory and Computation, 2009, 5, 1545-1553.	5.3	57
31	Symplectic integration and physical interpretation of time-dependent coupled-cluster theory. Journal of Chemical Physics, 2019, 150, 144106.	3.0	57
32	Systematic truncation of the virtual space in multiconfigurational perturbation theory. Journal of Chemical Physics, 2009, 131, 034113.	3.0	50
33	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.	3.0	48
34	Rovibrational structure of the Arâ€“CO complex based on a novel three-dimensional ab initio potential. Journal of Chemical Physics, 2002, 117, 6562-6572.	3.0	47
35	Redox Activity of Oxo-Bridged Iridium Dimers in an N,O-Donor Environment: Characterization of Remarkably Stable Ir(IV,V) Complexes. Journal of the American Chemical Society, 2017, 139, 9672-9683.	13.7	45
36	Dalton Project: A Python platform for molecular- and electronic-structure simulations of complex systems. Journal of Chemical Physics, 2020, 152, 214115.	3.0	45

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37	Thenâ†' Ï€* Electronic Transition in Microsolvated Formaldehyde. A Coupled Cluster and Combined Coupled Cluster/Molecular Mechanics Studyâ€. Journal of Physical Chemistry A, 2004, 108, 8624-8632.	2.5	44
38	On the importance of vibrational contributions to small-angle optical rotation: Fluoro-oxirane in gas phase and solution. Journal of Chemical Physics, 2009, 130, 034310.	3.0	43
39	Solvent Effects on Rotatory Strength Tensors. 1. Theory and Application of the Combined Coupled Cluster/Dielectric Continuum Model. Journal of Physical Chemistry A, 2004, 108, 3632-3641.	2.5	42
40	Quartic scaling evaluation of canonical scaled opposite spin second-order MÃ¸llerâ€“Plesset correlation energy using Cholesky decompositions. Chemical Physics Letters, 2007, 449, 354-357.	2.6	42
41	Spin flipping in ring-coupled-cluster-doubles theory. Chemical Physics Letters, 2011, 510, 147-153.	2.6	42
42	Communication: Analytic gradients in the random-phase approximation. Journal of Chemical Physics, 2013, 139, 081101.	3.0	38
43	Carbon Nanorings: A Challenge to Theoretical Chemistry. ChemPhysChem, 2006, 7, 2503-2507.	2.1	37
44	Gas phase optical rotation calculated from coupled cluster theory with zeroâ€point vibrational corrections from density functional theory. Chirality, 2009, 21, E68-75.	2.6	37
45	Gauge invariance of the coupled cluster oscillator strength. Chemical Physics Letters, 1998, 293, 251-260.	2.6	36
46	Origin invariant approaches to the calculation of two-photon circular dichroism. Journal of Chemical Physics, 2006, 125, 064113.	3.0	35
47	Coupled Cluster and MÃ¸llerâ€“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, 1921-1928.	5.3	35
48	Analytical gradients of the state-average complete active space self-consistent field method with density fitting. Journal of Chemical Physics, 2015, 143, 044110.	3.0	31
49	Computational and experimental investigation of intermolecular states and forces in the benzeneâ€“helium van der Waals complex. Journal of Chemical Physics, 2003, 119, 12956-12964.	3.0	30
50	Comparison of Three Efficient Approximate Exact-Exchange Algorithms: The Chain-of-Spheres Algorithm, Pair-Atomic Resolution-of-the-Identity Method, and Auxiliary Density Matrix Method. Journal of Chemical Theory and Computation, 2016, 12, 3514-3522.	5.3	29
51	Theoretical electronic absorption and natural circular dichroism spectra of (â^')-trans-cyclooctene. Journal of Chemical Physics, 2000, 112, 2139-2147.	3.0	26
52	On Resolution-of-the-Identity Electron Repulsion Integral Approximations and Variational Stability. Journal of Chemical Theory and Computation, 2017, 13, 4897-4906.	5.3	26
53	Analytical Gradients of Hartreeâ€“Fock Exchange with Density Fitting Approximations. Journal of Chemical Theory and Computation, 2013, 9, 204-212.	5.3	25
54	Numerical stability of time-dependent coupled-cluster methods for many-electron dynamics in intense laser pulses. Journal of Chemical Physics, 2020, 152, 071102.	3.0	25

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55	On the time-dependent Lagrangian approach in quantum chemistry. Journal of Chemical Physics, 1998, 108, 5194-5204.	3.0	24
56	Comment on â€œThe importance of high-order correlation effects for the COâ€“CO interaction potentialâ€• [Chem. Phys. Lett. 314 (1999) 326]. Chemical Physics Letters, 2001, 334, 419-423.	2.6	23
57	Polarizabilities of small annulenes from Cholesky CC2 linear response theory. Chemical Physics Letters, 2004, 390, 170-175.	2.6	23
58	Argon broadening of the 13CO R(0) and R(7) transitions in the fundamental band at temperatures between 80 and 297K: comparison between experiment and theory. Journal of Molecular Spectroscopy, 2003, 222, 131-141.	1.2	21
59	Role of the virtual orbitals and HOMO-LUMO gap in mean-field approximations to the conductance of molecular junctions. Physical Review B, 2008, 77, .	3.2	20
60	Analytical gradients of the second-order MÃ¸ller-Plesset energy using Cholesky decompositions. International Journal of Quantum Chemistry, 2014, 114, 321-327.	2.0	19
61	A coupled cluster study of the oriented circular dichroism of the nâ†'Ï€â^— electronic transition in cyclopropanone and natural optical active related structures. Chemical Physics Letters, 2004, 391, 259-266.	2.6	18
62	Interpretation of Coupled-Cluster Many-Electron Dynamics in Terms of Stationary States. Journal of Chemical Theory and Computation, 2021, 17, 388-404.	5.3	17
63	Study of the benzeneâ‹…N2 intermolecular potential-energy surface. Journal of Chemical Physics, 2003, 118, 1230-1241.	3.0	16
64	Variation of polarizability in the [4n + 2] annulene series: from [22]- to [66]-annulene. Physical Chemistry Chemical Physics, 2008, 10, 361-365.	2.8	15
65	Coupled cluster calculations of interaction energies in benzeneâ€“fluorobenzene van der Waals complexes. Chemical Physics Letters, 2007, 441, 332-335.	2.6	14
66	Ab initio potential-energy surface and rovibrational states of the HCNâ€“HCl complex. Journal of Chemical Physics, 2006, 124, 204315.	3.0	13
67	The CCSD(T) model with Cholesky decomposition of orbital energy denominators. International Journal of Quantum Chemistry, 2011, 111, 349-355.	2.0	11
68	Inner projection techniques for the low-cost handling of two-electron integrals in quantum chemistry. Molecular Physics, 2017, 115, 2052-2064.	1.7	11
69	Representation of the virtual space in extended systems â€“ a correlation energy convergence study. Molecular Physics, 2020, 118, e1733118.	1.7	10
70	Theoretical absorption spectrum of the Arâ€“CO van der Waals complex. Journal of Chemical Physics, 2003, 118, 9596-9607.	3.0	9
71	Divideâ€“Expandâ€“Consolidate Second-Order MÃ¸llerâ€“Plesset Theory with Periodic Boundary Conditions. Journal of Chemical Theory and Computation, 2018, 14, 2427-2438.	5.3	9
72	A molecule wired: Electrostatic investigation. Chemical Physics Letters, 2005, 405, 118-122.	2.6	8

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73	Design and synthesis of triazole-based peptidomimetics of a PSD-95 PDZ domain inhibitor. MedChemComm, 2016, 7, 531-536.	3.4	8
74	Linear and Nonlinear Optical Properties from TDOMP2 Theory. Journal of Chemical Theory and Computation, 2022, 18, 3687-3702.	5.3	8
75	Theoretical pressure and dielectric second virial coefficients of CO-Ar. Molecular Physics, 2008, 106, 881-892.	1.7	6
76	Introduction to Response Theory. , 2017, , 269-294.		4
77	Introduction to Response Theory. , 2012, , 135-156.		2
78	Introduction to Response Theory. , 2015, , 1-26.		2
79	Smooth potential-energy surfaces in fragmentation-based local correlation methods for periodic systems. Molecular Physics, 2021, 119, e1896046.	1.7	0