

Thomas B Pedersen

List of Publications by Citations

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78
papers

7,581
citations

38
h-index

79
g-index

79
ext. papers

8,244
ext. citations

4
avg, IF

5.54
L-index

#	Paper	IF	Citations
78	MOLCAS 7: the next generation. <i>Journal of Computational Chemistry</i> , 2010 , 31, 224-47	3.5	1425
77	Molcas 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. <i>Journal of Computational Chemistry</i> , 2016 , 37, 506-41	3.5	1047
76	The Dalton quantum chemistry program system. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2014 , 4, 269-284	7.9	956
75	Reduced scaling in electronic structure calculations using Cholesky decompositions. <i>Journal of Chemical Physics</i> , 2003 , 118, 9481-9484	3.9	342
74	Cholesky Decomposition-Based Multiconfiguration Second-Order Perturbation Theory (CD-CASPT2): Application to the Spin-State Energetics of Co(III)(diiminato)(NPh). <i>Journal of Chemical Theory and Computation</i> , 2008 , 4, 694-702	6.4	300
73	Low-cost evaluation of the exchange Fock matrix from Cholesky and density fitting representations of the electron repulsion integrals. <i>Journal of Chemical Physics</i> , 2007 , 126, 194106	3.9	256
72	Unbiased auxiliary basis sets for accurate two-electron integral approximations. <i>Journal of Chemical Physics</i> , 2007 , 127, 114107	3.9	228
71	Atomic Cholesky decompositions: a route to unbiased auxiliary basis sets for density fitting approximation with tunable accuracy and efficiency. <i>Journal of Chemical Physics</i> , 2009 , 130, 154107	3.9	160
70	Accurate ab initio density fitting for multiconfigurational self-consistent field methods. <i>Journal of Chemical Physics</i> , 2008 , 129, 024113	3.9	145
69	Origin invariant calculation of optical rotation without recourse to London orbitals. <i>Chemical Physics Letters</i> , 2004 , 393, 319-326	2.5	142
68	Density fitting with auxiliary basis sets from Cholesky decompositions. <i>Theoretical Chemistry Accounts</i> , 2009 , 124, 1-10	1.9	123
67	Fast noniterative orbital localization for large molecules. <i>Journal of Chemical Physics</i> , 2006 , 125, 174101	3.9	119
66	Modern quantum chemistry with [Open]Molcas. <i>Journal of Chemical Physics</i> , 2020 , 152, 214117	3.9	106
65	Polarizability and optical rotation calculated from the approximate coupled cluster singles and doubles CC2 linear response theory using Cholesky decompositions. <i>Journal of Chemical Physics</i> , 2004 , 120, 8887-97	3.9	99
64	Coupled cluster response functions revisited. <i>Journal of Chemical Physics</i> , 1997 , 106, 8059-8072	3.9	97
63	Coupled cluster calculations of the optical rotation of S-propylene oxide in gas phase and solution. <i>Chemical Physics Letters</i> , 2005 , 401, 385-392	2.5	92
62	Gauge invariant coupled cluster response theory. <i>Journal of Chemical Physics</i> , 1999 , 110, 8318-8327	3.9	87

61	The helium, neon, and argon cyclopropane van der Waals complexes: Ab initio ground state intermolecular potential energy surfaces and intermolecular dynamics. <i>Journal of Chemical Physics</i> , 2001 , 115, 8431-8439	3.9	78
60	Analytical State-Average Complete-Active-Space Self-Consistent Field Nonadiabatic Coupling Vectors: Implementation with Density-Fitted Two-Electron Integrals and Application to Conical Intersections. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 3636-53	6.4	75
59	Coupled cluster and density functional theory studies of the vibrational contribution to the optical rotation of (S)-propylene oxide. <i>Journal of the American Chemical Society</i> , 2006 , 128, 976-82	16.4	75
58	Calibration of Cholesky Auxiliary Basis Sets for Multiconfigurational Perturbation Theory Calculations of Excitation Energies. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 747-54	6.4	73
57	Gauge invariant coupled cluster response theory using optimized nonorthogonal orbitals. <i>Journal of Chemical Physics</i> , 2001 , 114, 6983-6993	3.9	73
56	Coupled cluster response calculation of natural chiroptical spectra. <i>Journal of Chemical Physics</i> , 1999 , 110, 2883-2892	3.9	72
55	MOLCAS [®] software for multiconfigurational quantum chemistry calculations. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2013 , 3, 143-149	7.9	61
54	Cholesky Decomposition Techniques in Electronic Structure Theory. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2011 , 301-343	0.7	61
53	Analytic derivatives for the Cholesky representation of the two-electron integrals. <i>Journal of Chemical Physics</i> , 2008 , 129, 034106	3.9	57
52	Ab initio calculation and display of the rotary strength tensor in the random phase approximation. Method and model studies. <i>Chemical Physics Letters</i> , 1995 , 246, 1-8	2.5	56
51	Attractive electron-electron interactions within robust local fitting approximations. <i>Journal of Computational Chemistry</i> , 2013 , 34, 1486-96	3.5	52
50	Ab Initio Density Fitting: Accuracy Assessment of Auxiliary Basis Sets from Cholesky Decompositions. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 1545-53	6.4	51
49	Orbital entanglement and CASSCF analysis of the Ru-NO bond in a Ruthenium nitrosyl complex. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 14383-92	3.6	49
48	Systematic truncation of the virtual space in multiconfigurational perturbation theory. <i>Journal of Chemical Physics</i> , 2009 , 131, 034113	3.9	45
47	Rovibrational structure of the Ar ⁺ O complex based on a novel three-dimensional ab initio potential. <i>Journal of Chemical Physics</i> , 2002 , 117, 6562-6572	3.9	45
46	The n-π* Electronic Transition in Microsolvated Formaldehyde. A Coupled Cluster and Combined Coupled Cluster/Molecular Mechanics Study. <i>Journal of Physical Chemistry A</i> , 2004 , 108, 8624-8632	2.8	43
45	Analytical gradients of complete active space self-consistent field energies using Cholesky decomposition: geometry optimization and spin-state energetics of a ruthenium nitrosyl complex. <i>Journal of Chemical Physics</i> , 2014 , 140, 174103	3.9	42
44	Spin flipping in ring-coupled-cluster-doubles theory. <i>Chemical Physics Letters</i> , 2011 , 510, 147-153	2.5	41

43	Solvent Effects on Rotatory Strength Tensors. 1. Theory and Application of the Combined Coupled Cluster/Dielectric Continuum Model. <i>Journal of Physical Chemistry A</i> , 2004 , 108, 3632-3641	2.8	41
42	On the importance of vibrational contributions to small-angle optical rotation: Fluoro-oxirane in gas phase and solution. <i>Journal of Chemical Physics</i> , 2009 , 130, 034310	3.9	40
41	Quartic scaling evaluation of canonical scaled opposite spin second-order Møller-Plesset correlation energy using Cholesky decompositions. <i>Chemical Physics Letters</i> , 2007 , 449, 354-357	2.5	38
40	Gas phase optical rotation calculated from coupled cluster theory with zero-point vibrational corrections from density functional theory. <i>Chirality</i> , 2009 , 21 Suppl 1, E68-75	2.1	36
39	Communication: Analytic gradients in the random-phase approximation. <i>Journal of Chemical Physics</i> , 2013 , 139, 081101	3.9	34
38	Redox Activity of Oxo-Bridged Iridium Dimers in an N,O-Donor Environment: Characterization of Remarkably Stable Ir(IV,V) Complexes. <i>Journal of the American Chemical Society</i> , 2017 , 139, 9672-9683	16.4	34
37	Carbon nanorings: A challenge to theoretical chemistry. <i>ChemPhysChem</i> , 2006 , 7, 2503-7	3.2	34
36	Coupled Cluster and Møller-Plesset Perturbation Theory Calculations of Noncovalent Intermolecular Interactions using Density Fitting with Auxiliary Basis Sets from Cholesky Decompositions. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 1921-8	6.4	32
35	Origin invariant approaches to the calculation of two-photon circular dichroism. <i>Journal of Chemical Physics</i> , 2006 , 125, 64113	3.9	32
34	Symplectic integration and physical interpretation of time-dependent coupled-cluster theory. <i>Journal of Chemical Physics</i> , 2019 , 150, 144106	3.9	29
33	Gauge invariance of the coupled cluster oscillator strength. <i>Chemical Physics Letters</i> , 1998 , 293, 251-260	2.5	29
32	Analytical gradients of the state-average complete active space self-consistent field method with density fitting. <i>Journal of Chemical Physics</i> , 2015 , 143, 044110	3.9	27
31	Computational and experimental investigation of intermolecular states and forces in the benzene-helium van der Waals complex. <i>Journal of Chemical Physics</i> , 2003 , 119, 12956-12964	3.9	27
30	Theoretical electronic absorption and natural circular dichroism spectra of (E)-trans-cyclooctene. <i>Journal of Chemical Physics</i> , 2000 , 112, 2139-2147	3.9	25
29	Dalton Project: A Python platform for molecular- and electronic-structure simulations of complex systems. <i>Journal of Chemical Physics</i> , 2020 , 152, 214115	3.9	24
28	Analytical Gradients of Hartree-Fock Exchange with Density Fitting Approximations. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 204-12	6.4	24
27	Comment on The importance of high-order correlation effects for the CO ₂ O interaction potential [Chem. Phys. Lett. 314 (1999) 326]. <i>Chemical Physics Letters</i> , 2001 , 334, 419-423	2.5	22
26	Polarizabilities of small annulenes from Cholesky CC2 linear response theory. <i>Chemical Physics Letters</i> , 2004 , 390, 170-175	2.5	21

25	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. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 3514-22	6.4	21
24	Argon broadening of the ^{13}CO R(0) and R(7) transitions in the fundamental band at temperatures between 80 and 297 K: comparison between experiment and theory. <i>Journal of Molecular Spectroscopy</i> , 2003 , 222, 131-141	1.3	19
23	On the time-dependent Lagrangian approach in quantum chemistry. <i>Journal of Chemical Physics</i> , 1998 , 108, 5194-5204	3.9	19
22	Analytical gradients of the second-order Møller-Plesset energy using Cholesky decompositions. <i>International Journal of Quantum Chemistry</i> , 2014 , 114, 321-327	2.1	18
21	A coupled cluster study of the oriented circular dichroism of the $n \rightarrow \pi^*$ electronic transition in cyclopropanone and natural optical active related structures. <i>Chemical Physics Letters</i> , 2004 , 391, 259-266	2.5	18
20	On Resolution-of-the-Identity Electron Repulsion Integral Approximations and Variational Stability. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 4897-4906	6.4	17
19	Role of the virtual orbitals and HOMO-LUMO gap in mean-field approximations to the conductance of molecular junctions. <i>Physical Review B</i> , 2008 , 77,	3.3	17
18	Study of the benzene- N_2 intermolecular potential-energy surface. <i>Journal of Chemical Physics</i> , 2003 , 118, 1230-1241	3.9	15
17	Variation of polarizability in the $[4n+2]$ annulene series: from $[22]$ - to $[66]$ -annulene. <i>Physical Chemistry Chemical Physics</i> , 2008 , 10, 361-5	3.6	14
16	Coupled cluster calculations of interaction energies in benzene-fluorobenzene van der Waals complexes. <i>Chemical Physics Letters</i> , 2007 , 441, 332-335	2.5	13
15	Numerical stability of time-dependent coupled-cluster methods for many-electron dynamics in intense laser pulses. <i>Journal of Chemical Physics</i> , 2020 , 152, 071102	3.9	11
14	Ab initio potential-energy surface and rovibrational states of the HCN-HCl complex. <i>Journal of Chemical Physics</i> , 2006 , 124, 204315	3.9	11
13	Inner projection techniques for the low-cost handling of two-electron integrals in quantum chemistry. <i>Molecular Physics</i> , 2017 , 115, 2052-2064	1.7	8
12	Design and synthesis of triazole-based peptidomimetics of a PSD-95 PDZ domain inhibitor. <i>MedChemComm</i> , 2016 , 7, 531-536	5	8
11	The CCSD(T) model with Cholesky decomposition of orbital energy denominators. <i>International Journal of Quantum Chemistry</i> , 2011 , 111, 349-355	2.1	8
10	Theoretical absorption spectrum of the Ar- O van der Waals complex. <i>Journal of Chemical Physics</i> , 2003 , 118, 9596-9607	3.9	8
9	A molecule wired: Electrostatic investigation. <i>Chemical Physics Letters</i> , 2005 , 405, 118-122	2.5	8
8	Theoretical pressure and dielectric second virial coefficients of CO_2 -Ar. <i>Molecular Physics</i> , 2008 , 106, 881-892	2	6

7	Representation of the virtual space in extended systems \mathbb{R}^3 correlation energy convergence study. <i>Molecular Physics</i> , 2020 , 118, e1733118	1.7	6
6	Interpretation of Coupled-Cluster Many-Electron Dynamics in Terms of Stationary States. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 388-404	6.4	5
5	Divide-Expand-Consolidate Second-Order Møller-Plesset Theory with Periodic Boundary Conditions. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 2427-2438	6.4	4
4	Introduction to Response Theory 2012 , 135-156		2
3	Introduction to Response Theory 2015 , 1-26		2
2	Introduction to Response Theory 2017 , 269-294		
1	Smooth potential-energy surfaces in fragmentation-based local correlation methods for periodic systems. <i>Molecular Physics</i> , 2021 , 119, e1896046	1.7	