Thomas B Pedersen

List of Publications by Year in Descending Order

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	Smooth potential-energy surfaces in fragmentation-based local correlation methods for periodic systems. *Molecular Physics*, **2021**, 119, e1896046	1.7	
77	Interpretation of Coupled-Cluster Many-Electron Dynamics in Terms of Stationary States. *Journal of Chemical Theory and Computation*, **2021**, 17, 388-404	6.4	5
76	Dalton Project: A Python platform for molecular- and electronic-structure simulations of complex systems. *Journal of Chemical Physics*, **2020**, 152, 214115	3.9	24
75	Modern quantum chemistry with [Open]Molcas. *Journal of Chemical Physics*, **2020**, 152, 214117	3.9	106
74	Numerical stability of time-dependent coupled-cluster methods for many-electron dynamics in intense laser pulses. *Journal of Chemical Physics*, **2020**, 152, 071102	3.9	11
73	Representation of the virtual space in extended systems a correlation energy convergence study. *Molecular Physics*, **2020**, 118, e1733118	1.7	6
72	Symplectic integration and physical interpretation of time-dependent coupled-cluster theory. *Journal of Chemical Physics*, **2019**, 150, 144106	3.9	29
71	Divide-Expand-Consolidate Second-Order M ller-Plesset Theory with Periodic Boundary Conditions. *Journal of Chemical Theory and Computation*, **2018**, 14, 2427-2438	6.4	4
70	Introduction to Response Theory **2017**, 269-294		
69	Inner projection techniques for the low-cost handling of two-electron integrals in quantum chemistry. *Molecular Physics*, **2017**, 115, 2052-2064	1.7	8
68	On Resolution-of-the-Identity Electron Repulsion Integral Approximations and Variational Stability. *Journal of Chemical Theory and Computation*, **2017**, 13, 4897-4906	6.4	17
67	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	16.4	34
66	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
65	Design and synthesis of triazole-based peptidomimetics of a PSD-95 PDZ domain inhibitor. *MedChemComm*, **2016**, 7, 531-536	5	8
64	Molcas 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. *Journal of Computational Chemistry*, **2016**, 37, 506-41	3.5	1047
63	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, 3514-22	6.4	21
62	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

61	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
60	Introduction to Response Theory **2015**, 1-26		2
59	The Dalton quantum chemistry program system. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 269-284	7.9	956
58	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
57	Analytical gradients of the second-order Møller-Plesset energy using Cholesky decompositions. *International Journal of Quantum Chemistry*, **2014**, 114, 321-327	2.1	18
56	Communication: Analytic gradients in the random-phase approximation. *Journal of Chemical Physics* , **2013**, 139, 081101	3.9	34
55	Analytical Gradients of Hartree-Fock Exchange with Density Fitting Approximations. *Journal of Chemical Theory and Computation*, **2013**, 9, 204-12	6.4	24
54	MOLCAS: software for multiconfigurational quantum chemistry calculations. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2013**, 3, 143-149	7.9	61
53	Attractive electron-electron interactions within robust local fitting approximations. *Journal of Computational Chemistry*, **2013**, 34, 1486-96	3.5	52
52	Coupled Cluster and Møller-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
51	Introduction to Response Theory **2012**, 135-156		2
50	The CCSD(T) model with Cholesky decomposition of orbital energy denominators. *International Journal of Quantum Chemistry*, **2011**, 111, 349-355	2.1	8
49	Spin flipping in ring-coupled-cluster-doubles theory. *Chemical Physics Letters*, **2011**, 510, 147-153	2.5	41
48	Cholesky Decomposition Techniques in Electronic Structure Theory. *Challenges and Advances in Computational Chemistry and Physics*, **2011**, 301-343	0.7	61
47	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
46	MOLCAS 7: the next generation. *Journal of Computational Chemistry*, **2010**, 31, 224-47	3.5	1425
45	Systematic truncation of the virtual space in multiconfigurational perturbation theory. *Journal of Chemical Physics*, **2009**, 131, 034113	3.9	45
44	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

43	Gas phase optical rotation calculated from coupled cluster theory with zero-point vibrational corrections from density funcional theory. *Chirality*, **2009**, 21 Suppl 1, E68-75	2.1	36
42	Density fitting with auxiliary basis sets from Cholesky decompositions. *Theoretical Chemistry Accounts*, **2009**, 124, 1-10	1.9	123
41	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
40	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	3.9	40
39	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	6.4	300
38	Analytic derivatives for the Cholesky representation of the two-electron integrals. *Journal of Chemical Physics*, **2008**, 129, 034106	3.9	57
37	Variation of polarizability in the [4n+2] annulene series: from [22]- to [66]-annulene. *Physical Chemistry Chemical Physics*, **2008**, 10, 361-5	3.6	14
36	Theoretical pressure and dielectric second virial coefficients of CO–Ar. *Molecular Physics*, **2008**, 106, 881-892	1.7	6
35	Accurate ab initio density fitting for multiconfigurational self-consistent field methods. *Journal of Chemical Physics*, **2008**, 129, 024113	3.9	145
34	Role of the virtual orbitals and HOMO-LUMO gap in mean-field approximations to the conductance of molecular junctions. *Physical Review B*, **2008**, 77,	3.3	17
33	Coupled cluster calculations of interaction energies in benzene–fluorobenzene van der Waals complexes. *Chemical Physics Letters*, **2007**, 441, 332-335	2.5	13
32	Quartic scaling evaluation of canonical scaled opposite spin second-order Møller–Plesset correlation energy using Cholesky decompositions. *Chemical Physics Letters*, **2007**, 449, 354-357	2.5	38
31	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
30	Unbiased auxiliary basis sets for accurate two-electron integral approximations. *Journal of Chemical Physics*, **2007**, 127, 114107	3.9	228
29	Carbon nanorings: A challenge to theoretical chemistry. *ChemPhysChem*, **2006**, 7, 2503-7	3.2	34
28	Origin invariant approaches to the calculation of two-photon circular dichroism. *Journal of Chemical Physics*, **2006**, 125, 64113	3.9	32
27	Fast noniterative orbital localization for large molecules. *Journal of Chemical Physics*, **2006**, 125, 174101	3.9	119
26	Ab initio potential-energy surface and rovibrational states of the HCN-HCl complex. *Journal of Chemical Physics*, **2006**, 124, 204315	3.9	11

25	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, 976-82	16.4	75
24	Coupled cluster calculations of the optical rotation of S-propylene oxide in gas phase and solution. *Chemical Physics Letters*, **2005**, 401, 385-392	2.5	92
23	A molecule wired: Electrostatic investigation. *Chemical Physics Letters*, **2005**, 405, 118-122	2.5	8
22	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, 8887-97	3.9	99
21	Polarizabilities of small annulenes from Cholesky CC2 linear response theory. *Chemical Physics Letters*, **2004**, 390, 170-175	2.5	21
20	A coupled cluster study of the oriented circular dichroism of the n-π* electronic transition in cyclopropanone and natural optical active related structures. *Chemical Physics Letters*, **2004**, 391, 259-266	2.5	18
19	Origin invariant calculation of optical rotation without recourse to London orbitals. *Chemical Physics Letters*, **2004**, 393, 319-326	2.5	142
18	The n -π* Electronic Transition in Microsolvated Formaldehyde. A Coupled Cluster and Combined Coupled Cluster/Molecular Mechanics Study *Journal of Physical Chemistry A*, **2004**, 108, 8624-8632	2.8	43
17	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	2.8	41
16	Argon broadening of the 13CO R(0) and R(7) transitions in the fundamental band at temperatures between 80 and 297 K: comparison between experiment and theory. *Journal of Molecular Spectroscopy*, **2003**, 222, 131-141	1.3	19
15	Reduced scaling in electronic structure calculations using Cholesky decompositions. *Journal of Chemical Physics*, **2003**, 118, 9481-9484	3.9	342
14	Study of the benzene?N2 intermolecular potential-energy surface. *Journal of Chemical Physics*, **2003**, 118, 1230-1241	3.9	15
13	Computational and experimental investigation of intermolecular states and forces in the benzene–helium van der Waals complex. *Journal of Chemical Physics*, **2003**, 119, 12956-12964	3.9	27
12	Theoretical absorption spectrum of the Ar–CO van der Waals complex. *Journal of Chemical Physics*, **2003**, 118, 9596-9607	3.9	8
11	Rovibrational structure of the Ar–CO complex based on a novel three-dimensional ab initio potential. *Journal of Chemical Physics*, **2002**, 117, 6562-6572	3.9	45
10	Comment on "The importance of high-order correlation effects for the CO–CO interaction potential" [Chem. Phys. Lett. 314 (1999) 326]. *Chemical Physics Letters*, **2001**, 334, 419-423	2.5	22
9	Gauge invariant coupled cluster response theory using optimized nonorthogonal orbitals. *Journal of Chemical Physics*, **2001**, 114, 6983-6993	3.9	73
8	The helium-, neon-, and argon–cyclopropane van der Waals complexes: Ab initio ground state intermolecular potential energy surfaces and intermolecular dynamics. *Journal of Chemical Physics*, **2001**, 115, 8431-8439	3.9	78

7	Theoretical electronic absorption and natural circular dichroism spectra of (l)-trans-cyclooctene. *Journal of Chemical Physics*, **2000**, 112, 2139-2147	3.9	25
6	Gauge invariant coupled cluster response theory. *Journal of Chemical Physics*, **1999**, 110, 8318-8327	3.9	87
5	Coupled cluster response calculation of natural chiroptical spectra. *Journal of Chemical Physics*, **1999**, 110, 2883-2892	3.9	72
4	Gauge invariance of the coupled cluster oscillator strength. *Chemical Physics Letters*, **1998**, 293, 251-260	2.5	29
3	On the time-dependent Lagrangian approach in quantum chemistry. *Journal of Chemical Physics*, **1998**, 108, 5194-5204	3.9	19
2	Coupled cluster response functions revisited. *Journal of Chemical Physics*, **1997**, 106, 8059-8072	3.9	97
1	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	2.5	56