Peter J Knowles

List of Publications by Year
in descending order

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110 papers	25,150 citations	43973 48 h-index	27345 106 g-index
113 all docs	113 docs citations	113 times ranked	7682 citing authors

#	Article	IF	Citations
1	An efficient internally contracted multiconfigurationâ€“reference configuration interaction method. Journal of Chemical Physics, 1988, 89, 5803-5814.	1.2	3,487
2	Molpro: a generalâ€purpose quantum chemistry program package. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 242-253.	6.2	2,852
3	A second order multiconfiguration SCF procedure with optimum convergence. Journal of Chemical Physics, 1985, 82, 5053-5063.	1.2	2,827
4	An efficient method for the evaluation of coupling coefficients in configuration interaction calculations. Chemical Physics Letters, 1988, 145, 514-522.	1.2	2,534
5	An efficient second-order MC SCF method for long configuration expansions. Chemical Physics Letters, 1985, 115, 259-267.	1.2	2,454
6	Coupled cluster theory for high spin, open shell reference wave functions. Journal of Chemical Physics, 1993, 99, 5219-5227.	1.2	1,878
7	Perturbative corrections to account for triple excitations in closed and open shell coupled cluster theories. Chemical Physics Letters, 1994, 227, 321-326.	1.2	982
8	Spin-orbit matrix elements for internally contracted multireference configuration interaction wavefunctions. Molecular Physics, 2000, 98, 1823-1833.	0.8	856
9	Fast linear scaling second-order MÃ¸ller-Plesset perturbation theory (MP2) using local and density fitting approximations. Journal of Chemical Physics, 2003, 118, 8149-8160.	1.2	652
10	The Molpro quantum chemistry package. Journal of Chemical Physics, 2020, 152, 144107.	1.2	603
11	Internally contracted multiconfiguration-reference configuration interaction calculations for excited states. Theoretica Chimica Acta, 1992, 84, 95-103.	0.9	504
12	High-Accuracy ab Initio Rotation-Vibration Transitions for Water. Science, 2003, 299, 539-542.	6.0	281
13	Fast Hartreeâ€“Fock theory using local density fitting approximations. Molecular Physics, 2004, 102, 2311-2321.	0.8	276
14	Restricted MÃ¸llerâ€”Plesset theory for open-shell molecules. Chemical Physics Letters, 1991, 186, 130-136.	1.2	265
15	A determinant based full configuration interaction program. Computer Physics Communications, 1989, 54, 75-83.	3.0	212
16	A comparison of variational and non-variational internally contracted multiconfiguration-reference configuration interaction calculations. Theoretica Chimica Acta, 1991, 78, 175-187.	0.9	175
17	Benchmark full configurationâ€interaction calculations on HF and NH2. Journal of Chemical Physics, 1986, 85, 1469-1474.	1.2	171
18	TheAâ€‰2Îâ€“Xâ€‰2Î£+red andBâ€‰2Î£+â€“Xâ€‰2Î£+violet systems of the CN radical: Accurate multireference configuration interaction calculations of the radiative transition probabilities. Journal of Chemical Physics, 1988, 89, 7334-7343.	1.2	151

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19	Open-shell Mâ^...llerâ€"Plesset perturbation theory. Chemical Physics Letters, 1991, 185, 256-264.	1.2	138
20	Slow convergence of the mÃ¸ller-plesset perturbation series: the dissociation energy of hydrogen cyanide and the electron affinity of the cyano radical. Chemical Physics Letters, 1987, 138, 481-485.	1.2	130
21	Improved radial grids for quadrature in molecular densityâ€functional calculations. Journal of Chemical Physics, 1996, 104, 9848-9858.	1.2	121
22	Unlimited full configuration interaction calculations. Journal of Chemical Physics, 1989, 91, 2396-2398.	1.2	107
23	Ab initio global potential, dipole, adiabatic, and relativistic correction surfaces for the HCNâ€"HNC system. Journal of Chemical Physics, 2001, 115, 3706-3718.	1.2	106
24	Benchmark studies of variational, unitary and extended coupled cluster methods. Journal of Chemical Physics, 2010, 133, 234102.	1.2	99
25	Insertion and Abstraction Pathways in the ReactionO(D21)+H2â†'OH+H. Physical Review Letters, 2001, 86, 1729-1732.	2.9	91
26	A comparative study of methods for describing non-adiabatic coupling: diabatic representation of the 1Î£+/1Î HOH and HHO conical intersections. Molecular Physics, 1997, 91, 1107-1123.	0.8	91
27	Projected unrestricted Mo/llerâ€"Plesset secondâ€order energies. Journal of Chemical Physics, 1988, 88, 6991-6998.	1.2	90
28	Analytic energy second derivatives for general MCSCF wave functions. Journal of Chemical Physics, 1984, 80, 2660-2668.	1.2	87
29	Theoretical assignment of the visible spectrum of singlet methylene. Journal of Chemical Physics, 1991, 94, 118-132.	1.2	84
30	Accurate multireference configuration interaction calculations of the potential energy function and the dissociation energy of N2. Journal of Chemical Physics, 1991, 94, 1264-1270.	1.2	83
31	Theoretical spinâ€"rovibronic 2A1(Îu)â€"2B1 spectrum of the H2O+, HDO+, and D2O+ cations. Journal of Chemical Physics, 1993, 98, 5222-5234.	1.2	77
32	A comparative study of methods for describing non-adiabatic coupling: diabatic representation of the 1Sigma +/1Pi HOH and HHO conical intersections. Molecular Physics, 1997, 91, 1107-1124.	0.8	77
33	Very large full configuration interaction calculations. Chemical Physics Letters, 1989, 155, 513-517.	1.2	76
34	Second-order MCSCF optimization revisited. I. Improved algorithms for fast and robust second-order CASSCF convergence. Journal of Chemical Physics, 2019, 150, 194106.	1.2	68
35	A full-CI study of the energetics of the reaction F + H2 â†' HF+H. Chemical Physics Letters, 1991, 185, 555-561.	1.2	65
36	A separable method for the calculation of dispersion and induction energy damping functions with applications to the dimers arising from He, Ne and HF. Molecular Physics, 1987, 60, 1143-1158.	0.8	63

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37	Convergence of projected unrestricted Hartee-Fock Moeller-Plesset series.. The Journal of Physical Chemistry, 1988, 92, 3097-3100.	2.9	63
38	Microwave electronic spectrum of the He+2 ion. Journal of Chemical Physics, 1995, 102, 5979-5988.	1.2	63
39	One-particle many-body Greenâ€™s function theory: Algebraic recursive definitions, linked-diagram theorem, irreducible-diagram theorem, and general-order algorithms. Journal of Chemical Physics, 2017, 147, 044108.	1.2	59
40	Polaritonic coupled-cluster theory. Physical Review Research, 2020, 2, .	1.3	57
41	Towards reliable modelling of large clusters: on the overall accuracy of the diatomics-in-molecule method for rare gas cluster ions. Chemical Physics, 1995, 193, 27-36.	0.9	55
42	Non-expanded dispersion and induction energies, and damping functions, for molecular interactions with application to HF-He. Molecular Physics, 1986, 59, 965-984.	0.8	52
43	Non-expanded dispersion energies and damping functions for Ar2 and Li2. Chemical Physics Letters, 1986, 124, 164-171.	1.2	50
44	Coupled ab initio potential energy surfaces for the reaction Cl(2P)+HClâ†'ClH+Cl(2P). Physical Chemistry Chemical Physics, 1999, 1, 957-966.	1.3	50
45	Ultrafast Photoinduced Dynamics of 1,3-Cyclohexadiene Using XMS-CASPT2 Surface Hopping. Journal of Chemical Theory and Computation, 2019, 15, 3929-3940.	2.3	50
46	On the assignment of the electronically excited singlet states in linear CO2. Chemical Physics Letters, 1988, 146, 230-235.	1.2	49
47	The 3.PI.8 .rarw. 3.SIGMA.u+ transition in nitrogen (N22+). The Journal of Physical Chemistry, 1991, 95, 2125-2127.	2.9	49
48	Quantum Tunneling Rates of Gas-Phase Reactions from On-the-Fly Instanton Calculations. Journal of Physical Chemistry Letters, 2016, 7, 4374-4379.	2.1	49
49	On the validity and applicability of the connected moments expansion. Chemical Physics Letters, 1987, 134, 512-518.	1.2	47
50	Convergence of Breitâ€“Pauli spinâ€“orbit matrix elements with basis set size and configuration interaction space: The halogen atoms F, Cl, and Br. Journal of Chemical Physics, 2000, 112, 5624-5632.	1.2	46
51	An Extended Computational Study of Criegee Intermediateâ€“Alcohol Reactions. Journal of Physical Chemistry A, 2019, 123, 218-229.	1.1	45
52	Spectroscopic and theoretical characterization of linear centrosymmetric Nâ‰¡Nâ‹…â‹…â‹…H+â‹…â‹…â‹…Nâ‰¡N. Journal of Chemical Physics, 1999, 111, 8400-8403.	1.2	44
53	Accurate numerical determination of Kohn-Sham potentials from electronic densities: I. Two-electron systems. Journal of Chemical Physics, 1997, 106, 9659-9667.	1.2	42
54	Approximate variational coupled cluster theory. Journal of Chemical Physics, 2011, 135, 044113.	1.2	41

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55	Quantemol Electron Collisions (QEC): An Enhanced Expert System for Performing Electron Molecule Collision Calculations Using the R-Matrix Method. Atoms, 2019, 7, 97.	0.7	41
56	Abinitiostudy of the energetics of the spinâ€allowed and spinâ€forbidden decomposition of HN3. Journal of Chemical Physics, 1990, 93, 3307-3318.	1.2	39
57	MCSCF optimization revisited. II. Combined first- and second-order orbital optimization for large molecules. Journal of Chemical Physics, 2020, 152, 074102.	1.2	38
58	Exchange energy in Kohn-Sham density-functional theory. Physical Review A, 1995, 51, 3571-3575.	1.0	36
59	The structures and stabilities of helium cluster ions. Molecular Physics, 1996, 87, 827-833.	0.8	36
60	Quasi-variational coupled cluster theory. Journal of Chemical Physics, 2012, 136, 054114.	1.2	35
61	An MCSCF study of the X 2 B 2, 2 A 2 and 2 2 B 2 states of benzyl. Journal of the Chemical Society, Faraday Transactions 2, 1987, 83, 1643.	1.1	31
62	High Accuracy ab Initio Calculations on Reactions of OH with 1-Alkenes. The Case of Propene. Journal of Chemical Theory and Computation, 2009, 5, 2313-2321.	2.3	31
63	Rigorously extensive orbital-invariant renormalized perturbative triples corrections from quasi-variational coupled cluster theory. Journal of Chemical Physics, 2013, 138, 074104.	1.2	31
64	Benchmark Quasi-Variational Coupled Cluster Calculations of Multiple Bond Breaking. Journal of Chemical Theory and Computation, 2012, 8, 2653-2660.	2.3	27
65	Ann-valued representation of He+npotentials. Molecular Physics, 1995, 85, 243-255.	0.8	26
66	Compressive sampling in configuration interaction wavefunctions. Molecular Physics, 2015, 113, 1655-1660.	0.8	26
67	Analytic nuclear forces and molecular properties from full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2015, 143, 054108.	1.2	24
68	Direct quantum dynamics using variational Gaussian wavepackets and Gaussian process regression. Journal of Chemical Physics, 2019, 150, 041101.	1.2	24
69	Parallel internally contracted multireference configuration interaction. , 1998, 19, 1215-1228.		21
70	Application of the quasi-variational coupled cluster method to the nonlinear optical properties of model hydrogen systems. Journal of Chemical Physics, 2012, 137, 054301.	1.2	20
71	Nonuniqueness of algebraic first-order density-matrix functionals. Physical Review A, 2015, 92, .	1.0	19
72	What Is the Price of Open-Source Software?. Journal of Physical Chemistry Letters, 2015, 6, 2751-2754.	2.1	19

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73	Theoretical photoabsorption spectrum of Ar3+. Chemical Physics Letters, 1999, 301, 241-247.	1.2	18
74	Breaking multiple covalent bonds with Hartreeâ€“Fock-based quantum chemistry: Quasi-Variational Coupled Cluster theory with perturbative treatment of triple excitations. Physical Chemistry Chemical Physics, 2012, 14, 6729.	1.3	18
75	Ab initio calculation of the Xâ€‰2Î£+ and Aâ€‰2Î states of CF++. Journal of Chemical Physics, 1990, 93, 562-569.	1.2	17
76	Theoretical photoabsorption spectra of Arn+ clusters. Chemical Physics Letters, 2000, 325, 648-654.	1.2	17
77	Ro-vibronic states of the NCS radical in the X2Î state. Physical Chemistry Chemical Physics, 1999, 1, 2649-2655.	1.3	16
78	A linked electron pair functional. Journal of Chemical Physics, 2010, 133, 224106.	1.2	15
79	Induced dipoleâ€"induced dipole interactions in Ar⁺_nclusters. Molecular Physics, 1999, 96, 749-755.	0.8	14
80	Multireferenceâ€"configuration interaction (MRî—¸CI) calculations of HS2+ and experimental observation via electron impact ionization of H2S. International Journal of Mass Spectrometry and Ion Processes, 1990, 100, 505-519.	1.9	12
81	Theoretical determination of the heat of formation of methylene. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 2025-2027.	1.7	12
82	Theoretical determination of the vibrational levels of NH+3and its isotopomers. Molecular Physics, 2001, 99, 1335-1346.	0.8	11
83	Symmetry dependence and universality of practical algebraic functionals in density-matrix-functional theory. Physical Review A, 2019, 99, .	1.0	11
84	Information entropy as a measure of the correlation energy associated with the cumulant. Physical Review A, 2021, 103, .	1.0	11
85	Theoretical rovibrational line intensities in the electronic ground state of ozone. Molecular Physics, 2004, 102, 2181-2189.	0.8	10
86	Statistical analysis of activation and reaction energies with quasi-variational coupled-cluster theory. Molecular Physics, 2018, 116, 1421-1427.	0.8	10
87	The metastable quartet state of He+4. Journal of Chemical Physics, 1995, 102, 9442-9443.	1.2	9
88	Generation of functional derivatives in Kohn-Sham density-functional theory. Computer Physics Communications, 1997, 100, 93-98.	3.0	9
89	Molecular second-quantized Hamiltonian: Electron correlation and non-adiabatic coupling treated on an equal footing. Journal of Chemical Physics, 2020, 153, 124102.	1.2	9
90	Quantum Chemistry in Dataflow: Density-Fitting MP2. Journal of Chemical Theory and Computation, 2017, 13, 5265-5272.	2.3	8

#	Article	IF	Citations
91	Parallel programming interface for distributed data. Computer Physics Communications, 2009, 180, 2673-2679.	3.0	7
92	The structures and stabilities of helium cluster ions. , 0, .		7
93	Polaritonic effects in the vibronic spectrum of molecules in an optical cavity. Journal of Chemical Physics, 2022, 156, .	1.2	6
94	Reply to â€œComment on â€œNonuniqueness of algebraic first-order density-matrix functionalsâ€â€‰â€• Physical Review A, 2018, 97, .	1.0	5
95	Quasi-variational coupled-cluster theory: Performance of perturbative treatments of connected triple excitations. Journal of Chemical Physics, 2018, 148, 194102.	1.2	5
96	Coupling electrons and vibrations in molecular quantum chemistry. Journal of Chemical Physics, 2020, 153, 214114.	1.2	5
97	Collins conjecture and information entropy in dissociating diatomic molecules. Physical Review A, 2021, 103, .	1.0	5
98	Low-lying electronic states of PH2+. Chemical Physics Letters, 1990, 175, 548-554.	1.2	4
99	Potential energy surfaces from Kohn-Sham potentials. Chemical Physics Letters, 1996, 262, 533-538.	1.2	4
100	Symbolic algebra in functional derivative potential calculations. , 1998, 19, 300-307.		4
101	Hans-Joachim Werner. Molecular Physics, 2010, 108, 221-222.	0.8	3
102	Perturbation-adapted perturbation theory. Journal of Chemical Physics, 2022, 156, 011101.	1.2	3
103	Improved version of parallel programming interface for distributed data with multiple helper servers. Computer Physics Communications, 2011, 182, 1502-1506.	3.0	2
104	Erratum to â€œGeneration of functional derivatives in Kohn-Sham density-functional theoryâ€•[Comput. Phys. Commun. 100 (1997) 93â€“98]. Computer Physics Communications, 1997, 103, 95-96.	3.0	1
105	Nicholas Charles Handy. 17 June 1941 â€” 2 October 2012. Biographical Memoirs of Fellows of the Royal Society, 2015, 61, 145-160.	0.1	1
106	Precise characterisation of isolated molecules: general discussion. Faraday Discussions, 2018, 212, 137-155.	1.6	1
107	The role of spinâ€“orbit effects in the mobility of N+ ions moving in a helium gas at low temperature. European Physical Journal D, 2020, 74, 1.	0.6	1
108	Electron Correlation in Small Molecules and the Configuration Interaction Method. , 1990, , 211-233.		1

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109	The determination of point groups from imprecise molecular geometries. Journal of Mathematical Chemistry, 2022, 60, 161-171.	0.7	1
110	Accurate Configuration Interaction Computations of Potential Energy Surfaces using Massively Parallel Computers. , 1999, , 237-248.		0