Peter J Knowles

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107 papers	21,986 citations	43 h-index	113 g-index
113 ext. papers	23,425 ext. citations	3.6 avg, IF	6.84 L-index

#	Paper	IF	Citations
107	An efficient internally contracted multiconfiguration–reference configuration interaction method. *Journal of Chemical Physics*, **1988**, 89, 5803-5814	3.9	3175
106	A second order multiconfiguration SCF procedure with optimum convergence. *Journal of Chemical Physics*, **1985**, 82, 5053-5063	3.9	2556
105	An efficient method for the evaluation of coupling coefficients in configuration interaction calculations. *Chemical Physics Letters*, **1988**, 145, 514-522	2.5	2327
104	Molpro: a general-purpose quantum chemistry program package. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 242-253	7.9	2254
103	An efficient second-order MC SCF method for long configuration expansions. *Chemical Physics Letters*, **1985**, 115, 259-267	2.5	2210
102	Coupled cluster theory for high spin, open shell reference wave functions. *Journal of Chemical Physics*, **1993**, 99, 5219-5227	3.9	1752
101	Perturbative corrections to account for triple excitations in closed and open shell coupled cluster theories. *Chemical Physics Letters*, **1994**, 227, 321-326	2.5	893
100	Spin-orbit matrix elements for internally contracted multireference configuration interaction wavefunctions. *Molecular Physics*, **2000**, 98, 1823-1833	1.7	741
99	Fast linear scaling second-order Møller-Plesset perturbation theory (MP2) using local and density fitting approximations. *Journal of Chemical Physics*, **2003**, 118, 8149-8160	3.9	606
98	Internally contracted multiconfiguration-reference configuration interaction calculations for excited states. *Theoretica Chimica Acta*, **1992**, 84, 95-103		436
97	High-accuracy ab initio rotation-vibration transitions for water. *Science*, **2003**, 299, 539-42	33.3	262
96	Fast Hartree–Fock theory using local density fitting approximations. *Molecular Physics*, **2004**, 102, 2311-2321	1.7	257
95	Restricted Møller–Plesset theory for open-shell molecules. *Chemical Physics Letters*, **1991**, 186, 130-136	2.5	239
94	The Molpro quantum chemistry package. *Journal of Chemical Physics*, **2020**, 152, 144107	3.9	197
93	A determinant based full configuration interaction program. *Computer Physics Communications*, **1989**, 54, 75-83	4.2	180
92	A comparison of variational and non-variational internally contracted multiconfiguration-reference configuration interaction calculations. *Theoretica Chimica Acta*, **1991**, 78, 175-187		166
91	Benchmark full configuration-interaction calculations on HF and NH2. *Journal of Chemical Physics*, **1986**, 85, 1469-1474	3.9	156

90	The A 2Σ+ 2Π red and B 2Π–X 2Π violet systems of the CN radical: Accurate multireference configuration interaction calculations of the radiative transition probabilities. *Journal of Chemical Physics*, **1988**, 89, 7334-7343	3.9	146
89	Slow convergence of the møller-plesset perturbation series: the dissociation energy of hydrogen cyanide and the electron affinity of the cyano radical. *Chemical Physics Letters*, **1987**, 138, 481-485	2.5	122
88	Open-shell M?llerPlesset perturbation theory. *Chemical Physics Letters*, **1991**, 185, 256-264	2.5	121
87	Improved radial grids for quadrature in molecular density-functional calculations. *Journal of Chemical Physics*, **1996**, 104, 9848-9858	3.9	107
86	Ab initio global potential, dipole, adiabatic, and relativistic correction surfaces for the HCNHNC system. *Journal of Chemical Physics*, **2001**, 115, 3706-3718	3.9	96
85	Unlimited full configuration interaction calculations. *Journal of Chemical Physics*, **1989**, 91, 2396-2398	3.9	94
84	Insertion and abstraction pathways in the reaction O(1D2) + H2-->OH+H. *Physical Review Letters*, **2001**, 86, 1729-32	7.4	88
83	Projected unrestricted Mo/llerPlesset second-order energies. *Journal of Chemical Physics*, **1988**, 88, 6991-6998	3.9	85
82	Analytic energy second derivatives for general MCSCF wave functions. *Journal of Chemical Physics*, **1984**, 80, 2660-2668	3.9	83
81	Accurate multireference configuration interaction calculations of the potential energy function and the dissociation energy of N2. *Journal of Chemical Physics*, **1991**, 94, 1264-1270	3.9	78
80	Theoretical assignment of the visible spectrum of singlet methylene. *Journal of Chemical Physics*, **1991**, 94, 118-132	3.9	77
79	Benchmark studies of variational, unitary and extended coupled cluster methods. *Journal of Chemical Physics*, **2010**, 133, 234102	3.9	74
78	Very large full configuration interaction calculations. *Chemical Physics Letters*, **1989**, 155, 513-517	2.5	74
77	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	1.7	73
76	Theoretical spinvibronic 2A1(Π)2B1 spectrum of the H2O+, HDO+, and D2O+ cations. *Journal of Chemical Physics*, **1993**, 98, 5222-5234	3.9	71
75	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	1.7	61
74	A full-CI study of the energetics of the reaction F + H2 -> HF+H. *Chemical Physics Letters*, **1991**, 185, 555-561	2.5	60
73	A comparative study of methods for describing non-adiabatic coupling: diabatic representation of the 1Π/1ΠHOH and HHO conical intersections. *Molecular Physics*, **1997**, 91, 1107-1123	1.7	60

72	Convergence of projected unrestricted Hartee-Fock Moeller-Plesset series.. *The Journal of Physical Chemistry*, **1988**, 92, 3097-3100		58
71	Microwave electronic spectrum of the He+2 ion. *Journal of Chemical Physics*, **1995**, 102, 5979-5988	3.9	55
70	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	2.3	53
69	Non-expanded dispersion energies and damping functions for Ar2 and Li2. *Chemical Physics Letters*, **1986**, 124, 164-171	2.5	47
68	Non-expanded dispersion and induction energies, and damping functions, for molecular interactions with application to HF-He. *Molecular Physics*, **1986**, 59, 965-984	1.7	46
67	The 3.PI.8 .rarw. 3.SIGMA.u+ transition in nitrogen (N22+). *The Journal of Physical Chemistry*, **1991**, 95, 2125-2127		45
66	Convergence of Breit□Pauli spin□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	3.9	43
65	Coupled abinitio potential energy surfaces for the reaction Cl(2P)+HCl->ClH+Cl(2P). *Physical Chemistry Chemical Physics*, **1999**, 1, 957-966	3.6	43
64	On the validity and applicability of the connected moments expansion. *Chemical Physics Letters*, **1987**, 134, 512-518	2.5	42
63	On the assignment of the electronically excited singlet states in linear CO2. *Chemical Physics Letters*, **1988**, 146, 230-235	2.5	42
62	One-particle many-body Green's function theory: Algebraic recursive definitions, linked-diagram theorem, irreducible-diagram theorem, and general-order algorithms. *Journal of Chemical Physics*, **2017**, 147, 044108	3.9	41
61	Quantum Tunneling Rates of Gas-Phase Reactions from On-the-Fly Instanton Calculations. *Journal of Physical Chemistry Letters*, **2016**, 7, 4374-4379	6.4	40
60	Approximate variational coupled cluster theory. *Journal of Chemical Physics*, **2011**, 135, 044113	3.9	40
59	Second-order MCSCF optimization revisited. I. Improved algorithms for fast and robust second-order CASSCF convergence. *Journal of Chemical Physics*, **2019**, 150, 194106	3.9	39
58	Accurate numerical determination of Kohn-Sham potentials from electronic densities: I. Two-electron systems. *Journal of Chemical Physics*, **1997**, 106, 9659-9667	3.9	39
57	Spectroscopic and theoretical characterization of linear centrosymmetric N?N??H+??N?N. *Journal of Chemical Physics*, **1999**, 111, 8400-8403	3.9	38
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54	Quasi-variational coupled cluster theory. *Journal of Chemical Physics*, **2012**, 136, 054114	3.9	33
53	The structures and stabilities of helium cluster ions. *Molecular Physics*, **1996**, 87, 827-833	1.7	31
52	Ultrafast Photoinduced Dynamics of 1,3-Cyclohexadiene Using XMS-CASPT2 Surface Hopping. *Journal of Chemical Theory and Computation*, **2019**, 15, 3929-3940	6.4	30
51	An Extended Computational Study of Criegee Intermediate-Alcohol Reactions. *Journal of Physical Chemistry A*, **2019**, 123, 218-229	2.8	30
50	Rigorously extensive orbital-invariant renormalized perturbative triples corrections from quasi-variational coupled cluster theory. *Journal of Chemical Physics*, **2013**, 138, 074104	3.9	29
49	An MCSCF study of the X2B2, 2A2 and 2 2B2 states of benzyl. *Journal of the Chemical Society, Faraday Transactions 2*, **1987**, 83, 1643		29
48	Benchmark Quasi-Variational Coupled Cluster Calculations of Multiple Bond Breaking. *Journal of Chemical Theory and Computation*, **2012**, 8, 2653-60	6.4	27
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46	Polaritonic coupled-cluster theory. *Physical Review Research*, **2020**, 2,	3.9	25
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44	An n-valued representation of He+ n potentials. *Molecular Physics*, **1995**, 85, 243-255	1.7	22
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40	Breaking multiple covalent bonds with Hartree-Fock-based quantum chemistry: Quasi-Variational Coupled Cluster theory with perturbative treatment of triple excitations. *Physical Chemistry Chemical Physics*, **2012**, 14, 6729-32	3.6	18
39	Parallel internally contracted multireference configuration interaction **1998**, 19, 1215-1228		18
38	Theoretical photoabsorption spectrum of Ar3+. *Chemical Physics Letters*, **1999**, 301, 241-247	2.5	18
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32	Ab initio calculation of the X 2□ and A 2□states of CF++. *Journal of Chemical Physics*, **1990**, 93, 562-569	3.9	14
31	Nonuniqueness of algebraic first-order density-matrix functionals. *Physical Review A*, **2015**, 92,	2.6	13
30	Multireference□onfiguration interaction (MR?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		12
29	Theoretical determination of the heat of formation ofmethylene. *Journal of the Chemical Society, Faraday Transactions*, **1997**, 93, 2025-2027		11
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19	Generation of functional derivatives in Kohn-Sham density-functional theory. *Computer Physics Communications*, **1997**, 100, 93-98	4.2	7

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16	Quasi-variational coupled-cluster theory: Performance of perturbative treatments of connected triple excitations. *Journal of Chemical Physics*, **2018**, 148, 194102	3.9	5
15	Reply to Comment on Nonuniqueness of algebraic first-order density-matrix functionals *Physical Review A*, **2018**, 97,	2.6	4
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7	Nicholas Charles Handy. 17 June 1941 2 October 2012. *Biographical Memoirs of Fellows of the Royal Society*, **2015**, 61, 145-160	0.1	1
6	Erratum to Generation of functional derivatives in Kohn-Sham density-functional theory [Comput. Phys. Commun. 100 (1997) 93 98]. *Computer Physics Communications*, **1997**, 103, 95-96	4.2	1
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4	Electron Correlation in Small Molecules and the Configuration Interaction Method **1990**, 211-233		1
3	The role of spin orbit effects in the mobility of N+ ions moving in a helium gas at low temperature. *European Physical Journal D*, **2020**, 74, 1	1.3	0
2	The determination of point groups from imprecise molecular geometries. *Journal of Mathematical Chemistry*, **2022**, 60, 161	2.1	
1	Accurate Configuration Interaction Computations of Potential Energy Surfaces using Massively Parallel Computers **1999**, 237-248		