Peter J Knowles

List of Publications by Year in Descending Order

Source: https://exaly.com/author-pdf/9411102/peter-j-knowles-publications-by-year.pdf
Version: 2024-04-20

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.
The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Perturbation-adapted perturbation theory.. *Journal of Chemical Physics*, **2022**, 156, 011101	3.9	1
106	The determination of point groups from imprecise molecular geometries. *Journal of Mathematical Chemistry*, **2022**, 60, 161	2.1	
105	Collins conjecture and information entropy in dissociating diatomic molecules. *Physical Review A*, **2021**, 103,	2.6	2
104	Information entropy as a measure of the correlation energy associated with the cumulant. *Physical Review A*, **2021**, 103,	2.6	2
103	MCSCF optimization revisited. II. Combined first- and second-order orbital optimization for large molecules. *Journal of Chemical Physics*, **2020**, 152, 074102	3.9	21
102	Polaritonic coupled-cluster theory. *Physical Review Research*, **2020**, 2,	3.9	25
101	Molecular second-quantized Hamiltonian: Electron correlation and non-adiabatic coupling treated on an equal footing. *Journal of Chemical Physics*, **2020**, 153, 124102	3.9	8
100	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
99	Coupling electrons and vibrations in molecular quantum chemistry. *Journal of Chemical Physics*, **2020**, 153, 214114	3.9	3
98	The Molpro quantum chemistry package. *Journal of Chemical Physics*, **2020**, 152, 144107	3.9	197
97	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
96	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
95	Symmetry dependence and universality of practical algebraic functionals in density-matrix-functional theory. *Physical Review A*, **2019**, 99,	2.6	7
94	Quantemol Electron Collisions (QEC): An Enhanced Expert System for Performing Electron Molecule Collision Calculations Using the R-Matrix Method. *Atoms*, **2019**, 7, 97	2.1	15
93	Direct quantum dynamics using variational Gaussian wavepackets and Gaussian process regression. *Journal of Chemical Physics*, **2019**, 150, 041101	3.9	18
92	An Extended Computational Study of Criegee Intermediate-Alcohol Reactions. *Journal of Physical Chemistry A*, **2019**, 123, 218-229	2.8	30
91	Reply to □Comment on □Nonuniqueness of algebraic first-order density-matrix functionals□□ *Physical Review A*, **2018**, 97,	2.6	4

90	Statistical analysis of activation and reaction energies with quasi-variational coupled-cluster theory. *Molecular Physics*, **2018**, 116, 1421-1427	1.7	10
89	Quasi-variational coupled-cluster theory: Performance of perturbative treatments of connected triple excitations. *Journal of Chemical Physics*, **2018**, 148, 194102	3.9	5
88	Quantum Chemistry in Dataflow: Density-Fitting MP2. *Journal of Chemical Theory and Computation*, **2017**, 13, 5265-5272	6.4	7
87	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
86	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
85	What Is the Price of Open-Source Software?. *Journal of Physical Chemistry Letters*, **2015**, 6, 2751-4	6.4	8
84	Analytic nuclear forces and molecular properties from full configuration interaction quantum Monte Carlo. *Journal of Chemical Physics*, **2015**, 143, 054108	3.9	18
83	Nonuniqueness of algebraic first-order density-matrix functionals. *Physical Review A*, **2015**, 92,	2.6	13
82	Nicholas Charles Handy. 17 June 1941 – 2 October 2012. *Biographical Memoirs of Fellows of the Royal Society*, **2015**, 61, 145-160	0.1	1
81	Compressive sampling in configuration interaction wavefunctions. *Molecular Physics*, **2015**, 113, 1655-1660	1.7	22
80	Rigorously extensive orbital-invariant renormalized perturbative triples corrections from quasi-variational coupled cluster theory. *Journal of Chemical Physics*, **2013**, 138, 074104	3.9	29
79	Benchmark Quasi-Variational Coupled Cluster Calculations of Multiple Bond Breaking. *Journal of Chemical Theory and Computation*, **2012**, 8, 2653-60	6.4	27
78	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
77	Molpro: a general-purpose quantum chemistry program package. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 242-253	7.9	2254
76	Application of the quasi-variational coupled cluster method to the nonlinear optical properties of model hydrogen systems. *Journal of Chemical Physics*, **2012**, 137, 054301	3.9	20
75	Quasi-variational coupled cluster theory. *Journal of Chemical Physics*, **2012**, 136, 054114	3.9	33
74	Approximate variational coupled cluster theory. *Journal of Chemical Physics*, **2011**, 135, 044113	3.9	40
73	Improved version of parallel programming interface for distributed data with multiple helper servers. *Computer Physics Communications*, **2011**, 182, 1502-1506	4.2	2

72	A linked electron pair functional. *Journal of Chemical Physics*, **2010**, 133, 224106	3.9	15
71	Benchmark studies of variational, unitary and extended coupled cluster methods. *Journal of Chemical Physics*, **2010**, 133, 234102	3.9	74
70	Parallel programming interface for distributed data. *Computer Physics Communications*, **2009**, 180, 2673-2679	4.6	7
69	High Accuracy ab Initio Calculations on Reactions of OH with 1-Alkenes. The Case of Propene. *Journal of Chemical Theory and Computation*, **2009**, 5, 2313-21	6.4	25
68	Theoretical rovibrational line intensities in the electronic ground state of ozone. *Molecular Physics*, **2004**, 102, 2181-2189	1.7	7
67	Fast Hartree–Fock theory using local density fitting approximations. *Molecular Physics*, **2004**, 102, 2311-2321	1.7	257
66	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
65	High-accuracy ab initio rotation-vibration transitions for water. *Science*, **2003**, 299, 539-42	33.3	262
64	Ab initio global potential, dipole, adiabatic, and relativistic correction surfaces for the HCN–HNC system. *Journal of Chemical Physics*, **2001**, 115, 3706-3718	3.9	96
63	Insertion and abstraction pathways in the reaction O(1D2) + H2-->OH+H. *Physical Review Letters*, **2001**, 86, 1729-32	7.4	88
62	Theoretical determination of the vibrational levels of NH+ 3 and its isotopomers. *Molecular Physics*, **2001**, 99, 1335-1346	1.7	11
61	Theoretical photoabsorption spectra of Arn+ clusters. *Chemical Physics Letters*, **2000**, 325, 648-654	2.5	17
60	Spin-orbit matrix elements for internally contracted multireference configuration interaction wavefunctions. *Molecular Physics*, **2000**, 98, 1823-1833	1.7	741
59	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
58	Spectroscopic and theoretical characterization of linear centrosymmetric N?N??H+??N?N. *Journal of Chemical Physics*, **1999**, 111, 8400-8403	3.9	38
57	Induced dipole–induced dipole interactions in Ar+ n clusters. *Molecular Physics*, **1999**, 96, 749-755	1.7	8
56	Theoretical photoabsorption spectrum of Ar3+. *Chemical Physics Letters*, **1999**, 301, 241-247	2.5	18
55	Ro-vibronic states of the NCS radical in the X2 state. *Physical Chemistry Chemical Physics*, **1999**, 1, 2649-2655	3.6	15

54	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
53	Accurate Configuration Interaction Computations of Potential Energy Surfaces using Massively Parallel Computers **1999**, 237-248		
52	Symbolic algebra in functional derivative potential calculations **1998**, 19, 300-307		4
51	Parallel internally contracted multireference configuration interaction **1998**, 19, 1215-1228		18
50	Theoretical determination of the heat of formation ofmethylene. *Journal of the Chemical Society, Faraday Transactions*, **1997**, 93, 2025-2027		11
49	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
48	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
47	Generation of functional derivatives in Kohn-Sham density-functional theory. *Computer Physics Communications*, **1997**, 100, 93-98	4.2	7
46	Erratum to □eneration of functional derivatives in Kohn-Sham density-functional theory□[Comput. Phys. Commun. 100 (1997) 93□8]. *Computer Physics Communications*, **1997**, 103, 95-96	4.2	1
45	A comparative study of methods for describing non-adiabatic coupling: diabatic representation of the 1□/1□HOH and HHO conical intersections. *Molecular Physics*, **1997**, 91, 1107-1123	1.7	60
44	The structures and stabilities of helium cluster ions. *Molecular Physics*, **1996**, 87, 827-833	1.7	31
43	Potential energy surfaces from Kohn-Sham potentials. *Chemical Physics Letters*, **1996**, 262, 533-538	2.5	4
42	Improved radial grids for quadrature in molecular density-functional calculations. *Journal of Chemical Physics*, **1996**, 104, 9848-9858	3.9	107
41	Exchange energy in Kohn-Sham density-functional theory. *Physical Review A*, **1995**, 51, 3571-3575	2.6	34
40	Microwave electronic spectrum of the He+2 ion. *Journal of Chemical Physics*, **1995**, 102, 5979-5988	3.9	55
39	An n-valued representation of He+ n potentials. *Molecular Physics*, **1995**, 85, 243-255	1.7	22
38	The metastable quartet state of He+4. *Journal of Chemical Physics*, **1995**, 102, 9442-9443	3.9	8
37	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

36	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
35	Coupled cluster theory for high spin, open shell reference wave functions. *Journal of Chemical Physics*, **1993**, 99, 5219-5227	3.9	1752
34	Theoretical spin□ovibronic 2A1(□)□2B1 spectrum of the H2O+, HDO+, and D2O+ cations. *Journal of Chemical Physics*, **1993**, 98, 5222-5234	3.9	71
33	Internally contracted multiconfiguration-reference configuration interaction calculations for excited states. *Theoretica Chimica Acta*, **1992**, 84, 95-103		436
32	Open-shell M?ller□lesset perturbation theory. *Chemical Physics Letters*, **1991**, 185, 256-264	2.5	121
31	Restricted M□ler□lesset theory for open-shell molecules. *Chemical Physics Letters*, **1991**, 186, 130-136	2.5	239
30	A full-CI study of the energetics of the reaction F + H2 -> HF+H. *Chemical Physics Letters*, **1991**, 185, 555-561	2.5	60
29	A comparison of variational and non-variational internally contracted multiconfiguration-reference configuration interaction calculations. *Theoretica Chimica Acta*, **1991**, 78, 175-187		166
28	The 3.PI.8 .rarw. 3.SIGMA.u+ transition in nitrogen (N22+). *The Journal of Physical Chemistry*, **1991**, 95, 2125-2127		45
27	Theoretical assignment of the visible spectrum of singlet methylene. *Journal of Chemical Physics*, **1991**, 94, 118-132	3.9	77
26	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
25	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
24	Ab initio study of the energetics of the spin-allowed and spin-forbidden decomposition of HN3. *Journal of Chemical Physics*, **1990**, 93, 3307-3318	3.9	35
23	Ab initio calculation of the X 2□ and A 2□states of CF++. *Journal of Chemical Physics*, **1990**, 93, 562-569	3.9	14
22	Low-lying electronic states of PH2+. *Chemical Physics Letters*, **1990**, 175, 548-554	2.5	4
21	Electron Correlation in Small Molecules and the Configuration Interaction Method **1990**, 211-233		1
20	Very large full configuration interaction calculations. *Chemical Physics Letters*, **1989**, 155, 513-517	2.5	74
19	A determinant based full configuration interaction program. *Computer Physics Communications*, **1989**, 54, 75-83	4.2	180

18	Unlimited full configuration interaction calculations. *Journal of Chemical Physics*, **1989**, 91, 2396-2398	3.9	94
17	An efficient method for the evaluation of coupling coefficients in configuration interaction calculations. *Chemical Physics Letters*, **1988**, 145, 514-522	2.5	2327
16	On the assignment of the electronically excited singlet states in linear CO2. *Chemical Physics Letters*, **1988**, 146, 230-235	2.5	42
15	An efficient internally contracted multiconfiguration□eference configuration interaction method. *Journal of Chemical Physics*, **1988**, 89, 5803-5814	3.9	3175
14	The A 2□ 2□ red and B 2□□ 2□ 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
13	Projected unrestricted Mo/ller□lesset second-order energies. *Journal of Chemical Physics*, **1988**, 88, 6991-6998	3.9	85
12	Convergence of projected unrestricted Hartee-Fock Moeller-Plesset series.. *The Journal of Physical Chemistry*, **1988**, 92, 3097-3100		58
11	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
10	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
9	Slow convergence of the m□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	2.5	122
8	On the validity and applicability of the connected moments expansion. *Chemical Physics Letters*, **1987**, 134, 512-518	2.5	42
7	Non-expanded dispersion energies and damping functions for Ar2 and Li2. *Chemical Physics Letters*, **1986**, 124, 164-171	2.5	47
6	Benchmark full configuration-interaction calculations on HF and NH2. *Journal of Chemical Physics*, **1986**, 85, 1469-1474	3.9	156
5	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
4	An efficient second-order MC SCF method for long configuration expansions. *Chemical Physics Letters*, **1985**, 115, 259-267	2.5	2210
3	A second order multiconfiguration SCF procedure with optimum convergence. *Journal of Chemical Physics*, **1985**, 82, 5053-5063	3.9	2556
2	Analytic energy second derivatives for general MCSCF wave functions. *Journal of Chemical Physics*, **1984**, 80, 2660-2668	3.9	83
1	The structures and stabilities of helium cluster ions		7