Alex J W Thom

List of Publications by Citations

45 papers	1,443 citations	17 h-index	37 g-index
53 ext. papers	1,771 ext. citations	5 avg, IF	5.11 L-index

#	Paper	IF	Citations
45	Fermion Monte Carlo without fixed nodes: a game of life, death, and annihilation in Slater determinant space. *Journal of Chemical Physics*, **2009**, 131, 054106	3.9	469
44	Breaking the carbon dimer: the challenges of multiple bond dissociation with full configuration interaction quantum Monte Carlo methods. *Journal of Chemical Physics*, **2011**, 135, 084104	3.9	120
43	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. *Journal of Chemical Physics*, **2021**, 155, 084801	3.9	115
42	LOBA: a localized orbital bonding analysis to calculate oxidation states, with application to a model water oxidation catalyst. *Physical Chemistry Chemical Physics*, **2009**, 11, 11297-304	3.6	81
41	Hartree-Fock solutions as a quasidiabatic basis for nonorthogonal configuration interaction. *Journal of Chemical Physics*, **2009**, 131, 124113	3.9	67
40	Locating multiple self-consistent field solutions: an approach inspired by metadynamics. *Physical Review Letters*, **2008**, 101, 193001	7.4	65
39	Stochastic coupled cluster theory. *Physical Review Letters*, **2010**, 105, 263004	7.4	64
38	Developments in stochastic coupled cluster theory: The initiator approximation and application to the uniform electron gas. *Journal of Chemical Physics*, **2016**, 144, 084108	3.9	35
37	Stochastic perturbation theory: a low-scaling approach to correlated electronic energies. *Physical Review Letters*, **2007**, 99, 143001	7.4	30
36	The HANDE-QMC Project: Open-Source Stochastic Quantum Chemistry from the Ground State Up. *Journal of Chemical Theory and Computation*, **2019**, 15, 1728-1742	6.4	29
35	Linked coupled cluster Monte Carlo. *Journal of Chemical Physics*, **2016**, 144, 044111	3.9	25
34	Stochastic coupled cluster theory: Efficient sampling of the coupled cluster expansion. *Journal of Chemical Physics*, **2017**, 147, 124105	3.9	23
33	Holomorphic Hartree-Fock Theory: An Inherently Multireference Approach. *Journal of Chemical Theory and Computation*, **2016**, 12, 167-73	6.4	21
32	A study of the dense uniform electron gas with high orders of coupled cluster. *Journal of Chemical Physics*, **2017**, 147, 194105	3.9	21
31	Open-Source Development Experiences in Scientific Software: The HANDE Quantum Monte Carlo Project. *Journal of Open Research Software*, **2015**, 3,	2.3	21
30	Holomorphic Hartree-Fock Theory and Configuration Interaction. *Journal of Chemical Theory and Computation*, **2014**, 10, 4795-800	6.4	18
29	Exciting Determinants in Quantum Monte Carlo: Loading the Dice with Fast, Low-Memory Weights. *Journal of Chemical Theory and Computation*, **2019**, 15, 127-140	6.4	17

28	Minimising biases in full configuration interaction quantum Monte Carlo. *Journal of Chemical Physics*, **2015**, 142, 104101	3.9	16
27	Holomorphic Hartree-Fock Theory: The Nature of Two-Electron Problems. *Journal of Chemical Theory and Computation*, **2018**, 14, 607-618	6.4	16
26	Preconditioning and Perturbative Estimators in Full Configuration Interaction Quantum Monte Carlo. *Journal of Chemical Theory and Computation*, **2019**, 15, 3537-3551	6.4	15
25	A combinatorial approach to the electron correlation problem. *Journal of Chemical Physics*, **2005**, 123, 204106	3.9	14
24	Diagrammatic Coupled Cluster Monte Carlo. *Journal of Physical Chemistry Letters*, **2019**, 10, 925-935	6.4	13
23	General Approach for Multireference Ground and Excited States Using Nonorthogonal Configuration Interaction. *Journal of Chemical Theory and Computation*, **2019**, 15, 4851-4861	6.4	13
22	Large scale parallelization in stochastic coupled cluster. *Journal of Chemical Physics*, **2018**, 149, 204103	3.9	13
21	Modeling Electron Transfers Using Quasidiabatic Hartree-Fock States. *Journal of Chemical Theory and Computation*, **2018**, 14, 4629-4639	6.4	12
20	Using SCF metadynamics to extend density matrix embedding theory to excited states. *Journal of Chemical Physics*, **2019**, 151, 034112	3.9	12
19	An Organic-Inorganic Hybrid Exhibiting Electrical Conduction and Single-Ion Magnetism. *Angewandte Chemie - International Edition*, **2020**, 59, 2399-2406	16.4	12
18	Complex adiabatic connection: A hidden non-Hermitian path from ground to excited states. *Journal of Chemical Physics*, **2019**, 150, 041103	3.9	11
17	Reaching Full Correlation through Nonorthogonal Configuration Interaction: A Second-Order Perturbative Approach. *Journal of Chemical Theory and Computation*, **2020**, 16, 5586-5600	6.4	11
16	Understanding and improving the efficiency of full configuration interaction quantum Monte Carlo. *Journal of Chemical Physics*, **2016**, 144, 094110	3.9	10
15	Accelerating Convergence in Fock Space Quantum Monte Carlo Methods. *Journal of Chemical Theory and Computation*, **2020**, 16, 1503-1510	6.4	7
14	Multireference Stochastic Coupled Cluster. *Journal of Chemical Theory and Computation*, **2019**, 15, 6625-6635	6.4	6
13	Symmetry in Multiple Self-Consistent-Field Solutions of Transition-Metal Complexes. *Journal of Chemical Theory and Computation*, **2020**, 16, 904-930	6.4	6
12	Parity-Time Symmetry in Hartree-Fock Theory. *Journal of Chemical Theory and Computation*, **2019**, 15, 4374-4385	6.4	5
11	Periodicity of Single-Molecule Magnet Behaviour of Heterotetranuclear Lanthanide Complexes across the Lanthanide Series: A Compendium. *Chemistry - A European Journal*, **2020**, 26, 6036-6049	4.8	5

10	A stochastic approach to unitary coupled cluster. *Journal of Chemical Physics*, **2020**, 153, 214106	3.9	5
9	Electron correlation from path resummations: the double-excitation star. *Physical Chemistry Chemical Physics*, **2008**, 10, 652-7	3.6	4
8	Ionic-caged heterometallic bismuth-platinum complex exhibiting electrocatalytic CO reduction. *Dalton Transactions*, **2020**, 49, 2652-2660	4.3	3
7	An Organic–Inorganic Hybrid Exhibiting Electrical Conduction and Single-Ion Magnetism. *Angewandte Chemie*, **2020**, 132, 2420-2427	3.6	3
6	Towards a Holomorphic Density Functional Theory. *Journal of Chemical Theory and Computation*, **2020**, 16, 7400-7412	6.4	2
5	New approaches to study excited states in density functional theory: general discussion. *Faraday Discussions*, **2020**, 224, 483-508	3.6	2
4	Theory and implementation of a novel stochastic approach to coupled cluster. *Journal of Chemical Physics*, **2020**, 153, 144117	3.9	2
3	Insight into the Gd–Pt Bond: Slow Magnetic Relaxation of a Heterometallic Gd–Pt Complex. *Bulletin of the Chemical Society of Japan*,	5.1	1
2	Field-programmable gate arrays and quantum Monte Carlo: Power efficient coprocessing for scalable high-performance computing. *International Journal of Quantum Chemistry*, **2019**, 119, e25853	2.1	0
1	Making the most of data: Quantum Monte Carlo postanalysis revisited.. *Physical Review E*, **2022**, 105, 045313	2.4	