

# Alex J W Thom

## List of Publications by Year in descending order

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Version: 2024-02-01

47  
papers

2,173  
citations

430874

18  
h-index

223800

46  
g-index

53  
all docs

53  
docs citations

53  
times ranked

1493  
citing authors

#	ARTICLE	IF	CITATIONS
1	Fermion Monte Carlo without fixed nodes: A game of life, death, and annihilation in Slater determinant space. <i>Journal of Chemical Physics</i> , 2009, 131, 054106.	3.0	567
2	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , 2021, 155, 084801.	3.0	518
3	LOBA: a localized orbital bonding analysis to calculate oxidation states, with application to a model water oxidation catalyst. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 11297.	2.8	134
4	Breaking the carbon dimer: The challenges of multiple bond dissociation with full configuration interaction quantum Monte Carlo methods. <i>Journal of Chemical Physics</i> , 2011, 135, 084104.	3.0	134
5	Hartree-Fock solutions as a quasidiabatic basis for nonorthogonal configuration interaction. <i>Journal of Chemical Physics</i> , 2009, 131, 124113.	3.0	90
6	Locating Multiple Self-Consistent Field Solutions: An Approach Inspired by Metadynamics. <i>Physical Review Letters</i> , 2008, 101, 193001.	7.8	74
7	Stochastic Coupled Cluster Theory. <i>Physical Review Letters</i> , 2010, 105, 263004.	7.8	71
8	Developments in stochastic coupled cluster theory: The initiator approximation and application to the uniform electron gas. <i>Journal of Chemical Physics</i> , 2016, 144, 084108.	3.0	40
9	The HANDE-QMC Project: Open-Source Stochastic Quantum Chemistry from the Ground State Up. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1728-1742.	5.3	33
10	Stochastic Perturbation Theory: A Low-Scaling Approach to Correlated Electronic Energies. <i>Physical Review Letters</i> , 2007, 99, 143001.	7.8	32
11	Holomorphic Hartree-Fock Theory: An Inherently Multireference Approach. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 167-173.	5.3	28
12	A study of the dense uniform electron gas with high orders of coupled cluster. <i>Journal of Chemical Physics</i> , 2017, 147, 194105.	3.0	28
13	Linked coupled cluster Monte Carlo. <i>Journal of Chemical Physics</i> , 2016, 144, 044111.	3.0	27
14	Stochastic coupled cluster theory: Efficient sampling of the coupled cluster expansion. <i>Journal of Chemical Physics</i> , 2017, 147, 124105.	3.0	26
15	Exciting Determinants in Quantum Monte Carlo: Loading the Dice with Fast, Low-Memory Weights. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 127-140.	5.3	24
16	Holomorphic Hartree-Fock Theory and Configuration Interaction. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4795-4800.	5.3	21
17	Open-Source Development Experiences in Scientific Software: The HANDE Quantum Monte Carlo Project. <i>Journal of Open Research Software</i> , 2015, 3, 9.	5.9	21
18	Preconditioning and Perturbative Estimators in Full Configuration Interaction Quantum Monte Carlo. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 3537-3551.	5.3	20

#	ARTICLE	IF	CITATIONS
19	An Organic-Inorganic Hybrid Exhibiting Electrical Conduction and Single-Ion Magnetism. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 2399-2406.	13.8	19
20	Minimising biases in full configuration interaction quantum Monte Carlo. <i>Journal of Chemical Physics</i> , 2015, 142, 104101.	3.0	18
21	Holomorphic Hartree-Fock Theory: The Nature of Two-Electron Problems. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 607-618.	5.3	18
22	Reaching Full Correlation through Nonorthogonal Configuration Interaction: A Second-Order Perturbative Approach. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 5586-5600.	5.3	18
23	A stochastic approach to unitary coupled cluster. <i>Journal of Chemical Physics</i> , 2020, 153, 214106.	3.0	17
24	Large scale parallelization in stochastic coupled cluster. <i>Journal of Chemical Physics</i> , 2018, 149, 204103.	3.0	15
25	Modeling Electron Transfers Using Quasidiabatic Hartree-Fock States. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4629-4639.	5.3	15
26	General Approach for Multireference Ground and Excited States Using Nonorthogonal Configuration Interaction. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4851-4861.	5.3	15
27	Using SCF metadynamics to extend density matrix embedding theory to excited states. <i>Journal of Chemical Physics</i> , 2019, 151, 034112.	3.0	15
28	A combinatorial approach to the electron correlation problem. <i>Journal of Chemical Physics</i> , 2005, 123, 204106.	3.0	14
29	Diagrammatic Coupled Cluster Monte Carlo. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 925-935.	4.6	14
30	Understanding and improving the efficiency of full configuration interaction quantum Monte Carlo. <i>Journal of Chemical Physics</i> , 2016, 144, 094110.	3.0	12
31	Complex adiabatic connection: A hidden non-Hermitian path from ground to excited states. <i>Journal of Chemical Physics</i> , 2019, 150, 041103.	3.0	12
32	Symmetry in Multiple Self-Consistent-Field Solutions of Transition-Metal Complexes. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 904-930.	5.3	11
33	Multireference Stochastic Coupled Cluster. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6625-6635.	5.3	10
34	Periodicity of Single-Molecule Magnet Behaviour of Heterotetranuclear Lanthanide Complexes across the Lanthanide Series: A Compendium. <i>Chemistry - A European Journal</i> , 2020, 26, 6036-6049.	3.3	9
35	Ionic-caged heterometallic bismuth-platinum complex exhibiting electrocatalytic CO <sub>2</sub> reduction. <i>Dalton Transactions</i> , 2020, 49, 2652-2660.	3.3	9
36	Accelerating Convergence in Fock Space Quantum Monte Carlo Methods. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 1503-1510.	5.3	7

#	ARTICLE	IF	CITATIONS
37	Parity-Time Symmetry in Hartree-Fock Theory. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4374-4385.	5.3	6
38	An Organic-Inorganic Hybrid Exhibiting Electrical Conduction and Single-Ion Magnetism. <i>Angewandte Chemie</i> , 2020, 132, 2420-2427.	2.0	5
39	Towards a Holomorphic Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7400-7412.	5.3	5
40	Electron correlation from path resummations: the double-excitation star. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 652-657.	2.8	4
41	Reducing unitary coupled cluster circuit depth by classical stochastic amplitude prescreening. <i>Physical Review Research</i> , 2022, 4, .	3.6	4
42	Theory and implementation of a novel stochastic approach to coupled cluster. <i>Journal of Chemical Physics</i> , 2020, 153, 144117.	3.0	3
43	Localized Spin Rotations: A Size-Consistent Approach to Nonorthogonal Configuration Interaction. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 710-722.	5.3	3
44	Insight into the Gd-Pt Bond: Slow Magnetic Relaxation of a Heterometallic Gd-Pt Complex. <i>Bulletin of the Chemical Society of Japan</i> , 2022, 95, 513-521.	3.2	3
45	New approaches to study excited states in density functional theory: general discussion. <i>Faraday Discussions</i> , 2020, 224, 483-508.	3.2	2
46	Field-programmable gate arrays and quantum Monte Carlo: Power efficient coprocessing for scalable high-performance computing. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25853.	2.0	1
47	Making the most of data: Quantum Monte Carlo postanalysis revisited. <i>Physical Review E</i> , 2022, 105, 045313.	2.1	1