Alex J W Thom

List of Publications by Year
in descending order

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47	2,173	430874	223800
papers	citations	18 h-index	46 g-index

53	53	53	1493
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Localized Spin Rotations: A Size-Consistent Approach to Nonorthogonal Configuration Interaction. Journal of Chemical Theory and Computation, 2022, 18, 710-722.	5.3	3
2	Insight into the Gdâ€“Pt Bond: Slow Magnetic Relaxation of a Heterometallic Gdâ€“Pt Complex. Bulletin of the Chemical Society of Japan, 2022, 95, 513-521.	3.2	3
3	Making the most of data: Quantum Monte Carlo postanalysis revisited. Physical Review E, 2022, 105, 045313.	2.1	1
4	Reducing unitary coupled cluster circuit depth by classical stochastic amplitude prescreening. Physical Review Research, 2022, 4, .	3.6	4
5	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	3.0	518
6	Symmetry in Multiple Self-Consistent-Field Solutions of Transition-Metal Complexes. Journal of Chemical Theory and Computation, 2020, 16, 904-930.	5.3	11
7	An Organicâ€“Inorganic Hybrid Exhibiting Electrical Conduction and Singleâ€Ion Magnetism. Angewandte Chemie, 2020, 132, 2420-2427.	2.0	5
8	An Organicâ€“Inorganic Hybrid Exhibiting Electrical Conduction and Singleâ€Ion Magnetism. Angewandte Chemie - International Edition, 2020, 59, 2399-2406.	13.8	19
9	Towards a Holomorphic Density Functional Theory. Journal of Chemical Theory and Computation, 2020, 16, 7400-7412.	5.3	5
10	New approaches to study excited states in density functional theory: general discussion. Faraday Discussions, 2020, 224, 483-508.	3.2	2
11	Reaching Full Correlation through Nonorthogonal Configuration Interaction: A Second-Order Perturbative Approach. Journal of Chemical Theory and Computation, 2020, 16, 5586-5600.	5.3	18
12	Theory and implementation of a novel stochastic approach to coupled cluster. Journal of Chemical Physics, 2020, 153, 144117.	3.0	3
13	Periodicity of Singleâ€Molecule Magnet Behaviour of Heterotetranuclear Lanthanide Complexes across the Lanthanide Series: A Compendium. Chemistry - A European Journal, 2020, 26, 6036-6049.	3.3	9
14	Accelerating Convergence in Fock Space Quantum Monte Carlo Methods. Journal of Chemical Theory and Computation, 2020, 16, 1503-1510.	5.3	7
15	Ionic-caged heterometallic bismuthâ€“platinum complex exhibiting electrocatalytic CO₂ reduction. Dalton Transactions, 2020, 49, 2652-2660.	3.3	9
16	A stochastic approach to unitary coupled cluster. Journal of Chemical Physics, 2020, 153, 214106.	3.0	17
17	General Approach for Multireference Ground and Excited States Using Nonorthogonal Configuration Interaction. Journal of Chemical Theory and Computation, 2019, 15, 4851-4861.	5.3	15
18	Using SCF metadynamics to extend density matrix embedding theory to excited states. Journal of Chemical Physics, 2019, 151, 034112.	3.0	15

#	Article	IF	Citations
19	Multireference Stochastic Coupled Cluster. Journal of Chemical Theory and Computation, 2019, 15, 6625-6635.	5.3	10
20	The HANDE-QMC Project: Open-Source Stochastic Quantum Chemistry from the Ground State Up. Journal of Chemical Theory and Computation, 2019, 15, 1728-1742.	5.3	33
21	Complex adiabatic connection: A hidden non-Hermitian path from ground to excited states. Journal of Chemical Physics, 2019, 150, 041103.	3.0	12
22	Parity-Time Symmetry in Hartreeâ€“Fock Theory. Journal of Chemical Theory and Computation, 2019, 15, 4374-4385.	5.3	6
23	Preconditioning and Perturbative Estimators in Full Configuration Interaction Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2019, 15, 3537-3551.	5.3	20
24	Fieldâ€programmable gate arrays and quantum Monte Carlo: Power efficient coprocessing for scalable highâ€performance computing. International Journal of Quantum Chemistry, 2019, 119, e25853.	2.0	1
25	Diagrammatic Coupled Cluster Monte Carlo. Journal of Physical Chemistry Letters, 2019, 10, 925-935.	4.6	14
26	Exciting Determinants in Quantum Monte Carlo: Loading the Dice with Fast, Low-Memory Weights. Journal of Chemical Theory and Computation, 2019, 15, 127-140.	5.3	24
27	Holomorphic Hartreeâ€“Fock Theory: The Nature of Two-Electron Problems. Journal of Chemical Theory and Computation, 2018, 14, 607-618.	5.3	18
28	Large scale parallelization in stochastic coupled cluster. Journal of Chemical Physics, 2018, 149, 204103.	3.0	15
29	Modeling Electron Transfers Using Quasidiabatic Hartreeâ€“Fock States. Journal of Chemical Theory and Computation, 2018, 14, 4629-4639.	5.3	15
30	Stochastic coupled cluster theory: Efficient sampling of the coupled cluster expansion. Journal of Chemical Physics, 2017, 147, 124105.	3.0	26
31	A study of the dense uniform electron gas with high orders of coupled cluster. Journal of Chemical Physics, 2017, 147, 194105.	3.0	28
32	Developments in stochastic coupled cluster theory: The initiator approximation and application to the uniform electron gas. Journal of Chemical Physics, 2016, 144, 084108.	3.0	40
33	Understanding and improving the efficiency of full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2016, 144, 094110.	3.0	12
34	Holomorphic Hartreeâ€“Fock Theory: An Inherently Multireference Approach. Journal of Chemical Theory and Computation, 2016, 12, 167-173.	5.3	28
35	Linked coupled cluster Monte Carlo. Journal of Chemical Physics, 2016, 144, 044111.	3.0	27
36	Minimising biases in full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2015, 142, 104101.	3.0	18

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37	Open-Source Development Experiences in Scientific Software: The HANDE Quantum Monte Carlo Project. Journal of Open Research Software, 2015, 3, 9.	5.9	21
38	Holomorphic Hartreeâ€“Fock Theory and Configuration Interaction. Journal of Chemical Theory and Computation, 2014, 10, 4795-4800.	5.3	21
39	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.	3.0	134
40	Stochastic Coupled Cluster Theory. Physical Review Letters, 2010, 105, 263004.	7.8	71
41	Fermion Monte Carlo without fixed nodes: A game of life, death, and annihilation in Slater determinant space. Journal of Chemical Physics, 2009, 131, 054106.	3.0	567
42	Hartreeâ€“Fock solutions as a quasidiabatic basis for nonorthogonal configuration interaction. Journal of Chemical Physics, 2009, 131, 124113.	3.0	90
43	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.	2.8	134
44	Electron correlation from path resummations: the double-excitation star. Physical Chemistry Chemical Physics, 2008, 10, 652-657.	2.8	4
45	Locating Multiple Self-Consistent Field Solutions: An Approach Inspired by Metadynamics. Physical Review Letters, 2008, 101, 193001.	7.8	74
46	Stochastic Perturbation Theory: A Low-Scaling Approach to Correlated Electronic Energies. Physical Review Letters, 2007, 99, 143001.	7.8	32
47	A combinatorial approach to the electron correlation problem. Journal of Chemical Physics, 2005, 123, 204106.	3.0	14