# Alex J W Thom

List of Publications by Year
in descending order



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|---|---|---|---|
| 47 papers | 2,173 citations | 430442 18 h-index | 223531 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. Journal of Chemical Physics, 2009, 131, 054106. | 1.2 | 567 |
| 2 | Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801. | 1.2 | 518 |
| 3 | 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. | 1.3 | 134 |
| 4 | 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. | 1.2 | 134 |
| 5 | Hartreeâ€“Fock solutions as a quasidiabatic basis for nonorthogonal configuration interaction. Journal of Chemical Physics, 2009, 131, 124113. | 1.2 | 90 |
| 6 | Locating Multiple Self-Consistent Field Solutions: An Approach Inspired by Metadynamics. Physical Review Letters, 2008, 101, 193001. | 2.9 | 74 |
| 7 | Stochastic Coupled Cluster Theory. Physical Review Letters, 2010, 105, 263004. | 2.9 | 71 |
| 8 | Developments in stochastic coupled cluster theory: The initiator approximation and application to the uniform electron gas. Journal of Chemical Physics, 2016, 144, 084108. | 1.2 | 40 |
| 9 | The HANDE-QMC Project: Open-Source Stochastic Quantum Chemistry from the Ground State Up. Journal of Chemical Theory and Computation, 2019, 15, 1728-1742. | 2.3 | 33 |
| 10 | Stochastic Perturbation Theory: A Low-Scaling Approach to Correlated Electronic Energies. Physical Review Letters, 2007, 99, 143001. | 2.9 | 32 |
| 11 | Holomorphic Hartreeâ€“Fock Theory: An Inherently Multireference Approach. Journal of Chemical Theory and Computation, 2016, 12, 167-173. | 2.3 | 28 |
| 12 | A study of the dense uniform electron gas with high orders of coupled cluster. Journal of Chemical Physics, 2017, 147, 194105. | 1.2 | 28 |
| 13 | Linked coupled cluster Monte Carlo. Journal of Chemical Physics, 2016, 144, 044111. | 1.2 | 27 |
| 14 | Stochastic coupled cluster theory: Efficient sampling of the coupled cluster expansion. Journal of Chemical Physics, 2017, 147, 124105. | 1.2 | 26 |
| 15 | Exciting Determinants in Quantum Monte Carlo: Loading the Dice with Fast, Low-Memory Weights. Journal of Chemical Theory and Computation, 2019, 15, 127-140. | 2.3 | 24 |
| 16 | Holomorphic Hartreeâ€“Fock Theory and Configuration Interaction. Journal of Chemical Theory and Computation, 2014, 10, 4795-4800. | 2.3 | 21 |
| 17 | Open-Source Development Experiences in Scientific Software: The HANDE Quantum Monte Carlo Project. Journal of Open Research Software, 2015, 3, 9. | 2.7 | 21 |
| 18 | Preconditioning and Perturbative Estimators in Full Configuration Interaction Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2019, 15, 3537-3551. | 2.3 | 20 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | An Organicâ€“Inorganic Hybrid Exhibiting Electrical Conduction and Singleâ€Ion Magnetism. Angewandte Chemie - International Edition, 2020, 59, 2399-2406. | 7.2 | 19 |
| 20 | Minimising biases in full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2015, 142, 104101. | 1.2 | 18 |
| 21 | Holomorphic Hartreeâ€“Fock Theory: The Nature of Two-Electron Problems. Journal of Chemical Theory and Computation, 2018, 14, 607-618. | 2.3 | 18 |
| 22 | Reaching Full Correlation through Nonorthogonal Configuration Interaction: A Second-Order Perturbative Approach. Journal of Chemical Theory and Computation, 2020, 16, 5586-5600. | 2.3 | 18 |
| 23 | A stochastic approach to unitary coupled cluster. Journal of Chemical Physics, 2020, 153, 214106. | 1.2 | 17 |
| 24 | Large scale parallelization in stochastic coupled cluster. Journal of Chemical Physics, 2018, 149, 204103. | 1.2 | 15 |
| 25 | Modeling Electron Transfers Using Quasidiabatic Hartreeâ€“Fock States. Journal of Chemical Theory and Computation, 2018, 14, 4629-4639. | 2.3 | 15 |
| 26 | General Approach for Multireference Ground and Excited States Using Nonorthogonal Configuration Interaction. Journal of Chemical Theory and Computation, 2019, 15, 4851-4861. | 2.3 | 15 |
| 27 | Using SCF metadynamics to extend density matrix embedding theory to excited states. Journal of Chemical Physics, 2019, 151, 034112. | 1.2 | 15 |
| 28 | A combinatorial approach to the electron correlation problem. Journal of Chemical Physics, 2005, 123, 204106. | 1.2 | 14 |
| 29 | Diagrammatic Coupled Cluster Monte Carlo. Journal of Physical Chemistry Letters, 2019, 10, 925-935. | 2.1 | 14 |
| 30 | Understanding and improving the efficiency of full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2016, 144, 094110. | 1.2 | 12 |
| 31 | Complex adiabatic connection: A hidden non-Hermitian path from ground to excited states. Journal of Chemical Physics, 2019, 150, 041103. | 1.2 | 12 |
| 32 | Symmetry in Multiple Self-Consistent-Field Solutions of Transition-Metal Complexes. Journal of Chemical Theory and Computation, 2020, 16, 904-930. | 2.3 | 11 |
| 33 | Multireference Stochastic Coupled Cluster. Journal of Chemical Theory and Computation, 2019, 15, 6625-6635. | 2.3 | 10 |
| 34 | Periodicity of Singleâ€Molecule Magnet Behaviour of Heterotetranuclear Lanthanide Complexes across the Lanthanide Series: A Compendium. Chemistry - A European Journal, 2020, 26, 6036-6049. | 1.7 | 9 |
| 35 | Ionic-caged heterometallic bismuthâ€“platinum complex exhibiting electrocatalytic CO<sub>2</sub> reduction. Dalton Transactions, 2020, 49, 2652-2660. | 1.6 | 9 |
| 36 | Accelerating Convergence in Fock Space Quantum Monte Carlo Methods. Journal of Chemical Theory and Computation, 2020, 16, 1503-1510. | 2.3 | 7 |

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|---|---|---|---|
| 37 | Parity-Time Symmetry in Hartreeâ€“Fock Theory. Journal of Chemical Theory and Computation, 2019, 15, 4374-4385. | 2.3 | 6 |
| 38 | An Organicâ€“Inorganic Hybrid Exhibiting Electrical Conduction and Singleâ€ion Magnetism. Angewandte Chemie, 2020, 132, 2420-2427. | 1.6 | 5 |
| 39 | Towards a Holomorphic Density Functional Theory. Journal of Chemical Theory and Computation, 2020, 16, 7400-7412. | 2.3 | 5 |
| 40 | Electron correlation from path resummations: the double-excitation star. Physical Chemistry Chemical Physics, 2008, 10, 652-657. | 1.3 | 4 |
| 41 | Reducing unitary coupled cluster circuit depth by classical stochastic amplitude prescreening. Physical Review Research, 2022, 4, . | 1.3 | 4 |
| 42 | Theory and implementation of a novel stochastic approach to coupled cluster. Journal of Chemical Physics, 2020, 153, 144117. | 1.2 | 3 |
| 43 | Localized Spin Rotations: A Size-Consistent Approach to Nonorthogonal Configuration Interaction. Journal of Chemical Theory and Computation, 2022, 18, 710-722. | 2.3 | 3 |
| 44 | 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. | 2.0 | 3 |
| 45 | New approaches to study excited states in density functional theory: general discussion. Faraday Discussions, 2020, 224, 483-508. | 1.6 | 2 |
| 46 | Fieldâ€programmable gate arrays and quantum Monte Carlo: Power efficient coprocessing for scalable highâ€performance computing. International Journal of Quantum Chemistry, 2019, 119, e25853. | 1.0 | 1 |
| 47 | Making the most of data: Quantum Monte Carlo postanalysis revisited. Physical Review E, 2022, 105, 045313. | 0.8 | 1 |