James Shee

List of Publications by Year
in descending order

22	715	567281 15	677142 22
papers	citations	h-index	g-index

29	29	29	634
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Calculation of Metallocene Ionization Potentials via Auxiliary Field Quantum Monte Carlo: Toward Benchmark Quantum Chemistry for Transition Metals. Journal of Chemical Theory and Computation, 2022, 18, 2845-2862.	5.3	18
2	A Localized-Orbital Energy Evaluation for Auxiliary-Field Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2022, 18, 3447-3459.	5.3	7
3	Concerted Electron-Nuclear Motion in Proton-Coupled Electron Transfer-Driven Grotthuss-Type Proton Translocation. Journal of Physical Chemistry Letters, 2022, , 4479-4485.	4.6	4
4	In silico prediction of annihilators for tripletâ€“triplet annihilation upconversion via auxiliary-field quantum Monte Carlo. Chemical Science, 2021, 12, 1068-1079.	7.4	7
5	Electronâ€“Nuclear Dynamics Accompanying Proton-Coupled Electron Transfer. Journal of the American Chemical Society, 2021, 143, 3104-3112.	13.7	21
6	Revealing the nature of electron correlation in transition metal complexes with symmetry breaking and chemical intuition. Journal of Chemical Physics, 2021, 154, 194109.	3.0	36
7	Regularized Second-Order MÃ¸llerâ€“Plesset Theory: A More Accurate Alternative to Conventional MP2 for Noncovalent Interactions and Transition Metal Thermochemistry for the Same Computational Cost. Journal of Physical Chemistry Letters, 2021, 12, 12084-12097.	4.6	32
8	Molecular Engineering of Chromophores to Enable Tripletâ€“Triplet Annihilation Upconversion. Journal of the American Chemical Society, 2020, 142, 19917-19925.	13.7	42
9	Predicting Excitation Energies of Twisted Intramolecular Charge-Transfer States with the Time-Dependent Density Functional Theory: Comparison with Experimental Measurements in the Gas Phase and Solvents Ranging from Hexanes to Acetonitrile. Journal of Chemical Theory and Computation, 2020, 16, 6244-6255.	5.3	21
10	The role of high-order electron correlation effects in a model system for non-valence correlation-bound anions. Journal of Chemical Physics, 2020, 153, 224118.	3.0	4
11	Solvent Mediated Excited State Proton Transfer in Indigo Carmine. Journal of Physical Chemistry Letters, 2020, 11, 4156-4162.	4.6	26
12	Multiple Stable Isopreneâ€“Ozone Complexes Reveal Complex Entrance Channel Dynamics in the Isoprene + Ozone Reaction. Journal of the American Chemical Society, 2020, 142, 10806-10813.	13.7	9
13	Accurate Quantum Chemical Calculation of Ionization Potentials: Validation of the DFT-LOC Approach via a Large Data Set Obtained from Experiments and Benchmark Quantum Chemical Calculations. Journal of Chemical Theory and Computation, 2020, 16, 2109-2123.	5.3	2
14	Predicting Ligand-Dissociation Energies of 3d Coordination Complexes with Auxiliary-Field Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2020, 16, 3041-3054.	5.3	21
15	Singletâ€“Triplet Energy Gaps of Organic Biradicals and Polyacenes with Auxiliary-Field Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2019, 15, 4924-4932.	5.3	37
16	Electrophotocatalysis with a Trisaminocyclopropenium Radical Dication. Angewandte Chemie, 2019, 131, 13452-13456.	2.0	43
17	Electrophotocatalysis with a Trisaminocyclopropenium Radical Dication. Angewandte Chemie - International Edition, 2019, 58, 13318-13322.	13.8	191
18	Efficient Ab Initio Auxiliary-Field Quantum Monte Carlo Calculations in Gaussian Bases via Low-Rank Tensor Decomposition. Journal of Chemical Theory and Computation, 2019, 15, 3510-3521.	5.3	39

#	Article	IF	Citations
19	On Achieving High Accuracy in Quantum Chemical Calculations of 3d Transition Metal-Containing Systems: A Comparison of Auxiliary-Field Quantum Monte Carlo with Coupled Cluster, Density Functional Theory, and Experiment for Diatomic Molecules. Journal of Chemical Theory and Computation, 2019, 15, 2346-2358.	5.3	62
20	Accurate Predictions of Electron Binding Energies of Dipole-Bound Anions via Quantum Monte Carlo Methods. Journal of Physical Chemistry Letters, 2018, 9, 6185-6190.	4.6	24
21	Phaseless Auxiliary-Field Quantum Monte Carlo on Graphical Processing Units. Journal of Chemical Theory and Computation, 2018, 14, 4109-4121.	5.3	35
22	Chemical Transformations Approaching Chemical Accuracy via Correlated Sampling in Auxiliary-Field Quantum Monte Carlo. Journal of Chemical Theory and Computation, 2017, 13, 2667-2680.	5.3	33