Shane M Parker

List of Publications by Year
in descending order

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21	1,155	566801 15	752256 20
papers	citations	h-index	g-index

22	22	22	1674
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Tuning the Properties of Azadipyrromethene-Based Near-Infrared Dyes Using Intramolecular BO Chelation and Peripheral Substitutions. Inorganic Chemistry, 2021, 60, 13320-13331.	1.9	11
2	Mutually Orthogonal Bioconjugation of Vinyl Nucleosides for RNA Metabolic Labeling. Organic Letters, 2021, 23, 7183-7187.	2.4	6
3	Accelerating molecular property calculations with semiempirical preconditioning. Journal of Chemical Physics, 2021, 155, 204111.	1.2	4
4	Surface hopping with cumulative probabilities: Even sampling and improved reproducibility. Journal of Chemical Physics, 2020, 153, 174109.	1.2	2
5	TURBOMOLE: Modular program suite for ab initio quantum-chemical and condensed-matter simulations. Journal of Chemical Physics, 2020, 152, 184107.	1.2	616
6	Expanding the Scope of RNA Metabolic Labeling with Vinyl Nucleosides and Inverse Electron-Demand Dielsâ€“Alder Chemistry. ACS Chemical Biology, 2019, 14, 1698-1707.	1.6	36
7	Multistate hybrid time-dependent density functional theory with surface hopping accurately captures ultrafast thymine photodeactivation. Physical Chemistry Chemical Physics, 2019, 21, 18999-19010.	1.3	31
8	Quadratic Response Properties from TDDFT: Trials and Tribulations. Journal of Chemical Theory and Computation, 2018, 14, 807-819.	2.3	49
9	Response Theory and Molecular Properties. , 2018, , 69-86.		5
10	Mechanism of photocatalytic water oxidation on small TiO₂ nanoparticles. Chemical Science, 2017, 8, 2179-2183.	3.7	59
11	Unphysical divergences in response theory. Journal of Chemical Physics, 2016, 145, 134105.	1.2	35
12	Orbital Optimization in the Active Space Decomposition Model. Journal of Chemical Theory and Computation, 2015, 11, 3636-3642.	2.3	15
13	Trinuclear tantalum clusters grafted to hydroxylated silica surfaces: A density-functional embedded-cluster study. Kinetics and Catalysis, 2015, 56, 631-639.	0.3	1
14	Communication: Active space decomposition with multiple sites: Density matrix renormalization group algorithm. Journal of Chemical Physics, 2014, 141, 211102.	1.2	38
15	Quasi-diabatic States from Active Space Decomposition. Journal of Chemical Theory and Computation, 2014, 10, 3738-3744.	2.3	27
16	Molecular Junctions: Can Pulling Influence Optical Controllability?. Nano Letters, 2014, 14, 4587-4591.	4.5	22
17	Model Hamiltonian Analysis of Singlet Fission from First Principles. Journal of Physical Chemistry C, 2014, 118, 12700-12705.	1.5	82
18	Olefin Hydrosilylation Catalyzed by a Bis-N-Heterocyclic Carbene Rhodium Complex. A Density Functional Theory Study. Organometallics, 2013, 32, 2363-2372.	1.1	18

#	Article	IF	Citations
19	Communication: Active-space decomposition for molecular dimers. Journal of Chemical Physics, 2013, 139, 021108.	1.2	48
20	Simulating strong field control of axial chirality using optimal control theory. Molecular Physics, 2012, 110, 1941-1952.	0.8	15
21	Coherent control of molecular torsion. Journal of Chemical Physics, 2011, 135, 224301.	1.2	35