Shane M Parker

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/2926737/publications.pdf

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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	TURBOMOLE: Modular program suite for ab initio quantum-chemical and condensed-matter simulations. Journal of Chemical Physics, 2020, 152, 184107.	1.2	616
2	Model Hamiltonian Analysis of Singlet Fission from First Principles. Journal of Physical Chemistry C, 2014, 118, 12700-12705.	1.5	82
3	Mechanism of photocatalytic water oxidation on small TiO₂ nanoparticles. Chemical Science, 2017, 8, 2179-2183.	3.7	59
4	Quadratic Response Properties from TDDFT: Trials and Tribulations. Journal of Chemical Theory and Computation, 2018, 14, 807-819.	2.3	49
5	Communication: Active-space decomposition for molecular dimers. Journal of Chemical Physics, 2013, 139, 021108.	1.2	48
6	Communication: Active space decomposition with multiple sites: Density matrix renormalization group algorithm. Journal of Chemical Physics, 2014, 141, 211102.	1.2	38
7	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
8	Coherent control of molecular torsion. Journal of Chemical Physics, 2011, 135, 224301.	1.2	35
9	Unphysical divergences in response theory. Journal of Chemical Physics, 2016, 145, 134105.	1.2	35
10	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
11	Quasi-diabatic States from Active Space Decomposition. Journal of Chemical Theory and Computation, 2014, 10, 3738-3744.	2.3	27
12	Molecular Junctions: Can Pulling Influence Optical Controllability?. Nano Letters, 2014, 14, 4587-4591.	4.5	22
13	Olefin Hydrosilylation Catalyzed by a Bis-N-Heterocyclic Carbene Rhodium Complex. A Density Functional Theory Study. Organometallics, 2013, 32, 2363-2372.	1.1	18
14	Simulating strong field control of axial chirality using optimal control theory. Molecular Physics, 2012, 110, 1941-1952.	0.8	15
15	Orbital Optimization in the Active Space Decomposition Model. Journal of Chemical Theory and Computation, 2015, 11, 3636-3642.	2.3	15
16	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
17	Mutually Orthogonal Bioconjugation of Vinyl Nucleosides for RNA Metabolic Labeling. Organic Letters, 2021, 23, 7183-7187.	2.4	6
18	Response Theory and Molecular Properties. , 2018, , 69-86.		5

#	Article	IF	Citations
19	Accelerating molecular property calculations with semiempirical preconditioning. Journal of Chemical Physics, 2021, 155, 204111.	1.2	4
20	Surface hopping with cumulative probabilities: Even sampling and improved reproducibility. Journal of Chemical Physics, 2020, 153, 174109.	1.2	2
21	Trinuclear tantalum clusters grafted to hydroxylated silica surfaces: A density-functional embedded-cluster study. Kinetics and Catalysis, 2015, 56, 631-639.	0.3	1