Samuel J Stoneburner

List of Publications by Year
in descending order

13 papers	493 citations	759233 12 h-index	1125743 13 g-index
13 all docs	13 docs citations	13 times ranked	913 citing authors

#	Article	IF	Citations
1	Automation of Active Space Selection for Multireference Methods via Machine Learning on Chemical Bond Dissociation. Journal of Chemical Theory and Computation, 2020, 16, 2389-2399.	5.3	40
2	Transition Metal Spin-State Energetics by MC-PDFT with High Local Exchange. Journal of Physical Chemistry A, 2020, 124, 1187-1195.	2.5	14
3	Beyond Density Functional Theory: The Multiconfigurational Approach To Model Heterogeneous Catalysis. ACS Catalysis, 2019, 9, 8481-8502.	11.2	75
4	Metalâ€“Organic Frameworks with Metalâ€“Catecholates for O₂/N₂ Separation. Journal of Physical Chemistry C, 2019, 123, 12935-12946.	3.1	33
5	Full Correlation in a Multiconfigurational Study of Bimetallic Clusters: Restricted Active Space Pair-Density Functional Theory Study of [2Feâ€“2S] Systems. Journal of Physical Chemistry C, 2019, 123, 11899-11907.	3.1	16
6	MC-PDFT can calculate singletâ€“triplet splittings of organic diradicals. Journal of Chemical Physics, 2018, 148, 064108.	3.0	30
7	Air Separation by Catechol-Ligated Transition Metals: A Quantum Chemical Screening. Journal of Physical Chemistry C, 2018, 122, 22345-22351.	3.1	16
8	Catechol-Ligated Transition Metals: A Quantum Chemical Study on a Promising System for Gas Separation. Journal of Physical Chemistry C, 2017, 121, 10463-10469.	3.1	20
9	Correction to â€œCatechol-Ligated Transition Metals: A Quantum Chemical Study on a Promising System for Gas Separationâ€. Journal of Physical Chemistry C, 2017, 121, 20553-20553.	3.1	1
10	Systematic design of active spaces for multi-reference calculations of singletâ€“triplet gaps of organic diradicals, with benchmarks against doubly electron-attached coupled-cluster data. Journal of Chemical Physics, 2017, 147, 164120.	3.0	20
11	Origin of the Strong Interaction between Polar Molecules and Copper(II) Paddle-Wheels in Metal Organic Frameworks. Journal of Physical Chemistry C, 2017, 121, 15135-15144.	3.1	23
12	Systematic Expansion of Active Spaces beyond the CASSCF Limit: A GASSCF/SplitGAS Benchmark Study. Journal of Chemical Theory and Computation, 2015, 11, 3010-3021.	5.3	48
13	Design of a Metalâ€“Organic Framework with Enhanced Back Bonding for Separation of N₂ and CH₄. Journal of the American Chemical Society, 2014, 136, 698-704.	13.7	157