Jonathan M Waldrop

List of Publications by Year in descending order

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1478505 1588992 9 659 6 8 citations h-index g-index papers 11 11 11 675 docs citations citing authors all docs times ranked

#	Article	IF	CITATIONS
1	From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape. Chemical Reviews, 2021, 121, 4962-4998.	47.7	39
2	Projector-Based Quantum Embedding for Molecular Systems: An Investigation of Three Partitioning Approaches. Journal of Physical Chemistry A, 2021, 125, 6384-6393.	2.5	9
3	Nonapproximated third-order exchange induction energy in symmetry-adapted perturbation theory. Journal of Chemical Physics, 2021, 154, 024103.	3.0	7
4	P <scp>SI4</scp> 1.4: Open-source software for high-throughput quantum chemistry. Journal of Chemical Physics, 2020, 152, 184108.	3.0	440
5	Interactions of CO ₂ with cluster models of <scp>metal–organic</scp> frameworks. Journal of Computational Chemistry, 2020, 41, 2066-2083.	3.3	O
6	Spin splittings from first-order symmetry-adapted perturbation theory without single-exchange approximation. Journal of Chemical Physics, 2019, 150, 074109.	3.0	9
7	Accurate virial coefficients of gaseous krypton from state-of-the-art <i>ab initio</i> potential and polarizability of the krypton dimer. Journal of Chemical Physics, 2018, 148, 024306.	3.0	4
8	P <scp>si</scp> 4N <scp>um</scp> P <scp>y</scp> : An Interactive Quantum Chemistry Programming Environment for Reference Implementations and Rapid Development. Journal of Chemical Theory and Computation, 2018, 14, 3504-3511.	5.3	106
9	Accurate <i>ab initio</i> potential for the krypton dimer and transport properties of the low-density krypton gas. Journal of Chemical Physics, 2015, 142, 204307.	3.0	33