

Jonathan M Waldrop

List of Publications by Year in descending order

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Version: 2024-02-01

9
papers

659
citations

1478505

6
h-index

1588992

8
g-index

11
all docs

11
docs citations

11
times ranked

675
citing authors

#	ARTICLE	IF	CITATIONS
1	P _{SI4} 1.4: Open-source software for high-throughput quantum chemistry. Journal of Chemical Physics, 2020, 152, 184108.	3.0	440
2	P _{si4Nump} : 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
3	From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape. Chemical Reviews, 2021, 121, 4962-4998.	47.7	39
4	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
5	Spin splittings from first-order symmetry-adapted perturbation theory without single-exchange approximation. Journal of Chemical Physics, 2019, 150, 074109.	3.0	9
6	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
7	Nonapproximated third-order exchange induction energy in symmetry-adapted perturbation theory. Journal of Chemical Physics, 2021, 154, 024103.	3.0	7
8	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
9	Interactions of CO ₂ with cluster models of metal-organic frameworks. Journal of Computational Chemistry, 2020, 41, 2066-2083.	3.3	0