Ashutosh Kumar

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	<scp>Psi4</scp> 1.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and Interoperability. Journal of Chemical Theory and Computation, 2017, 13, 3185-3197.	5.3	961
2	P <scp>SI4</scp> 1.4: Open-source software for high-throughput quantum chemistry. Journal of Chemical Physics, 2020, 152, 184108.	3.0	440
3	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
4	Quantum simulation of electronic structure with a transcorrelated Hamiltonian: improved accuracy with a smaller footprint on the quantum computer. Physical Chemistry Chemical Physics, 2020, 22, 24270-24281.	2.8	43
5	Frozen Virtual Natural Orbitals for Coupled-Cluster Linear-Response Theory. Journal of Physical Chemistry A, 2017, 121, 708-716.	2.5	40
6	Reducedâ€scaling coupled cluster response theory: Challenges and opportunities. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1406.	14.6	26
7	Massively Parallel Quantum Chemistry: A high-performance research platform for electronic structure. Journal of Chemical Physics, 2020, 153, 044120.	3.0	25
8	Explicitly correlated coupled cluster method for accurate treatment of open-shell molecules with hundreds of atoms. Journal of Chemical Physics, 2020, 153, 094105.	3.0	22
9	Many-Body Quantum Chemistry on Massively Parallel Computers. Chemical Reviews, 2021, 121, 1203-1231.	47.7	21
10	Frozen-Density Embedding Potentials and Chiroptical Properties. Journal of Chemical Theory and Computation, 2015, 11, 5305-5315.	5.3	16
11	Incremental evaluation of coupled cluster dipole polarizabilities. Physical Chemistry Chemical	2.8	13