## **Romit Chakraborty**

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	3.0	518
2	Ambient-Temperature Hydrogen Storage via Vanadium(II)-Dihydrogen Complexation in a Metal–Organic Framework. Journal of the American Chemical Society, 2021, 143, 6248-6256.	13.7	81
3	Generalized Pauli conditions on the spectra of one-electron reduced density matrices of atoms and molecules. Physical Review A, 2014, 89, .	2.5	47
4	Observation of an Intermediate to H <sub>2</sub> Binding in a Metal–Organic Framework. Journal of the American Chemical Society, 2021, 143, 14884-14894.	13.7	32
5	Sufficient condition for the openness of a many-electron quantum system from the violation of a generalized Pauli exclusion principle. Physical Review A, 2015, 91, .	2.5	26
6	Structure of the oneâ€electron reduced density matrix from the generalized <scp>P</scp> auli exclusion principle. International Journal of Quantum Chemistry, 2015, 115, 1305-1310.	2.0	20
7	Role of the generalized pauli constraints in the quantum chemistry of excited states. International Journal of Quantum Chemistry, 2016, 116, 784-790.	2.0	15
8	Quantum Chemical Modeling of Pressureâ€Induced Spin Crossover in Octahedral Metalâ€Ligand Complexes. ChemPhysChem, 2019, 20, 2742-2747.	2.1	14
9	Noise-assisted energy transfer from the dilation of the set of one-electron reduced density matrices. Journal of Chemical Physics, 2017, 146, 184101.	3.0	12
10	Sparsity of the wavefunction from the generalized Pauli exclusion principle. Journal of Chemical Physics, 2018, 148, 054106.	3.0	10
11	Variational aspects of the Klein–Gordon equation. Indian Journal of Physics, 2015, 89, 181-187.	1.8	2