Saswata Dasgupta

List of Publications by Year
in descending order

10 papers	745 citations	1162367 8 h-index	1372195 10 g-index
12 all docs	12 docs citations	12 times ranked	570 citing authors

#	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.	1.2	518
2	Standard grids for highâ€precision integration of modern density functionals: SGâ€2 and SGâ€3. Journal of Computational Chemistry, 2017, 38, 869-882.	1.5	70
3	Elevating density functional theory to chemical accuracy for water simulations through a density-corrected many-body formalism. Nature Communications, 2021, 12, 6359.	5.8	45
4	General Many-Body Framework for Data-Driven Potentials with Arbitrary Quantum Mechanical Accuracy: Water as a Case Study. Journal of Chemical Theory and Computation, 2021, 17, 5635-5650.	2.3	28
5	Ab Initio Investigation of the Resonance Raman Spectrum of the Hydrated Electron. Journal of Physical Chemistry B, 2019, 123, 8074-8085.	1.2	25
6	How Good Is the Density-Corrected SCAN Functional for Neutral and Ionic Aqueous Systems, and What Is So Right about the Hartreeâ€“Fock Density?. Journal of Chemical Theory and Computation, 2022, 18, 4745-4761.	2.3	20
7	Assessing the Interplay between Functional-Driven and Density-Driven Errors in DFT Models of Water. Journal of Chemical Theory and Computation, 2022, 18, 3410-3426.	2.3	14
8	Using Atomic Confining Potentials for Geometry Optimization and Vibrational Frequency Calculations in Quantum-Chemical Models of Enzyme Active Sites. Journal of Physical Chemistry B, 2020, 124, 1137-1147.	1.2	11
9	Density functional theory of water with the machine-learned DM21 functional. Journal of Chemical Physics, 2022, 156, 161103.	1.2	8
10	Ab InitioApproach to Femtosecond Stimulated Raman Spectroscopy: Investigating Vibrational Modes Probed in Excited-State Relaxation of Quaterthiophenes. Journal of Physical Chemistry A, 2020, 124, 6356-6362.	1.1	1