

Saswata Dasgupta

List of Publications by Year in descending order

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Version: 2024-02-01

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	Density functional theory of water with the machine-learned DM21 functional. <i>Journal of Chemical Physics</i> , 2022, 156, 161103.	1.2	8
2	Assessing the Interplay between Functional-Driven and Density-Driven Errors in DFT Models of Water. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3410-3426.	2.3	14
3	How Good Is the Density-Corrected SCAN Functional for Neutral and Ionic Aqueous Systems, and What Is So Right about the Hartree-Fock Density?. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 4745-4761.	2.3	20
4	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , 2021, 155, 084801.	1.2	518
5	General Many-Body Framework for Data-Driven Potentials with Arbitrary Quantum Mechanical Accuracy: Water as a Case Study. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5635-5650.	2.3	28
6	Elevating density functional theory to chemical accuracy for water simulations through a density-corrected many-body formalism. <i>Nature Communications</i> , 2021, 12, 6359.	5.8	45
7	<i>Ab Initio</i> Approach to Femtosecond Stimulated Raman Spectroscopy: Investigating Vibrational Modes Probed in Excited-State Relaxation of Quaterthiophenes. <i>Journal of Physical Chemistry A</i> , 2020, 124, 6356-6362.	1.1	1
8	Using Atomic Confining Potentials for Geometry Optimization and Vibrational Frequency Calculations in Quantum-Chemical Models of Enzyme Active Sites. <i>Journal of Physical Chemistry B</i> , 2020, 124, 1137-1147.	1.2	11
9	<i>Ab Initio</i> Investigation of the Resonance Raman Spectrum of the Hydrated Electron. <i>Journal of Physical Chemistry B</i> , 2019, 123, 8074-8085.	1.2	25
10	Standard grids for high-precision integration of modern density functionals: SG-2 and SG-3. <i>Journal of Computational Chemistry</i> , 2017, 38, 869-882.	1.5	70