

Soumen Ghosh

List of Publications by Year in descending order

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Version: 2024-02-01

18
papers

1,109
citations

758635

12
h-index

839053

18
g-index

23
all docs

23
docs citations

23
times ranked

1806
citing authors

#	ARTICLE	IF	CITATIONS
1	Origin of the Failure of Density Functional Theories in Predicting Inverted Singlet-Triplet Gaps. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1378-1385.	1.1	24
2	Near-Quantitative Predictions of the First-Shell Coordination Structure of Hydrated First-Row Transition Metal Ions Using K-Edge X-ray Absorption Near-Edge Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 6323-6330.	2.1	6
3	Fragment-Based Local Coupled Cluster Embedding Approach for the Quantification and Analysis of Noncovalent Interactions: Exploring the Many-Body Expansion of the Local Coupled Cluster Energy. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3348-3359.	2.3	7
4	Addressing the System-Size Dependence of the Local Approximation Error in Coupled-Cluster Calculations. <i>Journal of Physical Chemistry A</i> , 2021, 125, 9932-9939.	1.1	17
5	A new density for transition properties within the similarity transformed equation of motion approach. <i>Molecular Physics</i> , 2020, 118, e1818858.	0.8	3
6	NWChem: Past, present, and future. <i>Journal of Chemical Physics</i> , 2020, 152, 184102.	1.2	425
7	Revised M11 Exchange-Correlation Functional for Electronic Excitation Energies and Ground-State Properties. <i>Journal of Physical Chemistry A</i> , 2019, 123, 2966-2990.	1.1	76
8	A semiempirical effective Hamiltonian based approach for analyzing excited state wave functions and computing excited state absorption spectra using real-time dynamics. <i>Journal of Chemical Physics</i> , 2019, 150, 104103.	1.2	10
9	Synthesis and Characterization of Electron-Deficient Asymmetrically Substituted Diarylindenotetracenes. <i>Journal of Organic Chemistry</i> , 2018, 83, 1828-1841.	1.7	10
10	Combining Wave Function Methods with Density Functional Theory for Excited States. <i>Chemical Reviews</i> , 2018, 118, 7249-7292.	23.0	166
11	Generalized-active-space pair-density functional theory: an efficient method to study large, strongly correlated, conjugated systems. <i>Chemical Science</i> , 2017, 8, 2741-2750.	3.7	60
12	Partial Fluorination as a Strategy for Crystal Engineering of Rubrene Derivatives. <i>Crystal Growth and Design</i> , 2017, 17, 643-658.	1.4	24
13	Modeling Optical Spectra of Large Organic Systems Using Real-Time Propagation of Semiempirical Effective Hamiltonians. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4410-4420.	2.3	16
14	Charge Transport in 4 nm Molecular Wires with Interrupted Conjugation: Combined Experimental and Computational Evidence for Thermally Assisted Polaron Tunneling. <i>ACS Nano</i> , 2016, 10, 4372-4383.	7.3	56
15	Multiconfiguration Pair-Density Functional Theory Is as Accurate as CASPT2 for Electronic Excitation. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 586-591.	2.1	75
16	Multiconfiguration Pair-Density Functional Theory Outperforms Kohn-Sham Density Functional Theory and Multireference Perturbation Theory for Ground-State and Excited-State Charge Transfer. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3643-3649.	2.3	40
17	Length-Dependent Nanotransport and Charge Hopping Bottlenecks in Long Thiophene-Containing π -Conjugated Molecular Wires. <i>Journal of the American Chemical Society</i> , 2015, 137, 15732-15741.	6.6	76
18	Enhancing the double exchange interaction in a mixed valence {VIII-VII} pair: a theoretical perspective. <i>Dalton Transactions</i> , 2013, 42, 16490.	1.6	18