Soumen Ghosh

List of Publications by Year
in descending order

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18	1,109	758635 12	839053 18
papers	citations	h-index	g-index

23	23	23	1806
all docs	docs citations	times ranked	citing authors

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