

Soumen Saha

List of Publications by Year in descending order

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Version: 2024-02-01

21
papers

768
citations

567281

15
h-index

677142

22
g-index

23
all docs

23
docs citations

23
times ranked

671
citing authors

#	ARTICLE	IF	CITATIONS
1	Sequence Analysis, Structure Prediction of Receptor Proteins and In Silico Study of Potential Inhibitors for Management of Life Threatening COVID-19. <i>Letters in Drug Design and Discovery</i> , 2022, 19, 108-122.	0.7	1
2	Towards developing a criterion to characterize non-covalent bonds: a quantum mechanical study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 8478-8488.	2.8	29
3	Theoretically predicting the feasibility of highly-fluorinated ethers as promising diluents for non-flammable concentrated electrolytes. <i>Scientific Reports</i> , 2020, 10, 21966.	3.3	6
4	Microscopic Origin of the Solid Electrolyte Interphase Formation in Fire-Extinguishing Electrolyte: Formation of Pure Inorganic Layer in High Salt Concentration. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 5949-5955.	4.6	15
5	Probing the Most Stable Isomer of Zirconium Bis(phenoxy-imine) Cation: A Computational Investigation. <i>Journal of Physical Chemistry A</i> , 2018, 122, 2198-2208.	2.5	3
6	Differential cationization of fatty acids with monovalent cations studied by electrospray ionization tandem mass spectrometry and a computational approach. <i>Rapid Communications in Mass Spectrometry</i> , 2018, 32, 1126-1134.	1.5	2
7	On the origin of spurious errors in many-body expansion for water cluster. <i>Journal of Chemical Sciences</i> , 2017, 129, 1053-1060.	1.5	3
8	Palladium-Catalyzed Tandem-Cyclization of Functionalized Ynamides: An Approach to Benzosultams. <i>Advanced Synthesis and Catalysis</i> , 2016, 358, 1625-1638.	4.3	36
9	Cooperative or Anticooperative: How Noncovalent Interactions Influence Each Other. <i>Journal of Physical Chemistry B</i> , 2015, 119, 11121-11135.	2.6	66
10	Quantifying cooperativity in water clusters: an attempt towards obtaining a generalised equation. <i>Molecular Physics</i> , 2015, 113, 3031-3041.	1.7	16
11	DFT-based reactivity study of (5,5) armchair boron nitride nanotube (BNNT). <i>Chemical Physics Letters</i> , 2013, 565, 69-73.	2.6	39
12	Hardness potential derivatives and their relation to Fukui indices. <i>Journal of Computational Chemistry</i> , 2013, 34, 662-672.	3.3	18
13	Open and capped (5,5) armchair SWCNTs: A comparative study of DFT-based reactivity descriptors. <i>Chemical Physics Letters</i> , 2012, 541, 85-91.	2.6	46
14	Surface Reactivity for Chlorination on Chlorinated (5,5) Armchair SWCNT: A Computational Approach. <i>Journal of Physical Chemistry C</i> , 2012, 116, 22399-22410.	3.1	62
15	On the complementarity of comprehensive decomposition analysis of stabilization energy (CDASE) – Scheme and supermolecular approach. <i>Chemical Physics</i> , 2012, 394, 29-35.	1.9	46
16	CDASE – A reliable scheme to explain the reactivity sequence between Diels-Alder pairs. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 9328.	2.8	58
17	Studies of regioselectivity of large molecular systems using DFT based reactivity descriptors. <i>Annual Reports on the Progress of Chemistry Section C</i> , 2010, 106, 118.	4.4	84
18	Are the Hirshfeld and Mulliken population analysis schemes consistent with chemical intuition?. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 1790-1806.	2.0	102

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19	A comprehensive decomposition analysis of stabilization energy (CDASE) and its application in locating the rate-determining step of multi-step reactions. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 8306.	2.8	63
20	N-Dependence problem of local hardness parameter. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 5591.	2.8	26
21	“One-into-Many” Model: An Approach on DFT Based Reactivity Descriptor to Predict the Regioselectivity of Large Systems. <i>Journal of Physical Chemistry B</i> , 2007, 111, 9664-9674.	2.6	32