

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 | Are the Hirshfeld and Mulliken population analysis schemes consistent with chemical intuition?. International Journal of Quantum Chemistry, 2009, 109, 1790-1806. | 2.0 | 102 |
| 2 | Studies of regioselectivity of large molecular systems using DFT based reactivity descriptors. Annual Reports on the Progress of Chemistry Section C, 2010, 106, 118. | 4.4 | 84 |
| 3 | Cooperative or Anticooperative: How Noncovalent Interactions Influence Each Other. Journal of Physical Chemistry B, 2015, 119, 11121-11135. | 2.6 | 66 |
| 4 | A comprehensive decomposition analysis of stabilization energy (CDASE) and its application in locating the rate-determining step of multi-step reactions. Physical Chemistry Chemical Physics, 2009, 11, 8306. | 2.8 | 63 |
| 5 | Surface Reactivity for Chlorination on Chlorinated (5,5) Armchair SWCNT: A Computational Approach. Journal of Physical Chemistry C, 2012, 116, 22399-22410. | 3.1 | 62 |
| 6 | CDASE—A reliable scheme to explain the reactivity sequence between Diels—Alder pairs. Physical Chemistry Chemical Physics, 2010, 12, 9328. | 2.8 | 58 |
| 7 | Open and capped (5,5) armchair SWCNTs: A comparative study of DFT-based reactivity descriptors. Chemical Physics Letters, 2012, 541, 85-91. | 2.6 | 46 |
| 8 | On the complementarity of comprehensive decomposition analysis of stabilization energy (CDASE) —Scheme and supermolecular approach. Chemical Physics, 2012, 394, 29-35. | 1.9 | 46 |
| 9 | DFT-based reactivity study of (5,5) armchair boron nitride nanotube (BNNT). Chemical Physics Letters, 2013, 565, 69-73. | 2.6 | 39 |
| 10 | Palladium—Catalyzed Tandem—Cyclization of Functionalized Ynamides: An Approach to Benzosultams. Advanced Synthesis and Catalysis, 2016, 358, 1625-1638. | 4.3 | 36 |
| 11 | —One-into-Many—Model:— An Approach on DFT Based Reactivity Descriptor to Predict the Regioselectivity of Large Systems. Journal of Physical Chemistry B, 2007, 111, 9664-9674. | 2.6 | 32 |
| 12 | Towards developing a criterion to characterize non-covalent bonds: a quantum mechanical study. Physical Chemistry Chemical Physics, 2021, 23, 8478-8488. | 2.8 | 29 |
| 13 | N-Dependence problem of local hardness parameter. Physical Chemistry Chemical Physics, 2008, 10, 5591. | 2.8 | 26 |
| 14 | Hardness potential derivatives and their relation to Fukui indices. Journal of Computational Chemistry, 2013, 34, 662-672. | 3.3 | 18 |
| 15 | Quantifying cooperativity in water clusters: an attempt towards obtaining a generalised equation. Molecular Physics, 2015, 113, 3031-3041. | 1.7 | 16 |
| 16 | Microscopic Origin of the Solid Electrolyte Interphase Formation in Fire-Extinguishing Electrolyte: Formation of Pure Inorganic Layer in High Salt Concentration. Journal of Physical Chemistry Letters, 2019, 10, 5949-5955. | 4.6 | 15 |
| 17 | Theoretically predicting the feasibility of highly-fluorinated ethers as promising diluents for non-flammable concentrated electrolytes. Scientific Reports, 2020, 10, 21966. | 3.3 | 6 |
| 18 | On the origin of spurious errors in many-body expansion for water cluster. Journal of Chemical Sciences, 2017, 129, 1053-1060. | 1.5 | 3 |

| # | ARTICLE | IF | CITATIONS |
|----|---|-----|-----------|
| 19 | 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 |
| 20 | 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 |
| 21 | 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 |