

Subrahmanyam Sappati

List of Publications by Year in descending order

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Version: 2024-02-01

15
papers

212
citations

1163117

8
h-index

996975

15
g-index

16
all docs

16
docs citations

16
times ranked

372
citing authors

#	ARTICLE	IF	CITATIONS
1	Ab-initio investigations for structural, mechanical, optoelectronic, and thermoelectric properties of Ba ₂ SbXO ₆ (X Nb, Ta) compounds. <i>Journal of Alloys and Compounds</i> , 2022, 893, 162332.	5.5	7
2	Reverse vaccinology-based prediction of a multi-epitope SARS-CoV-2 vaccine and its tailoring to new coronavirus variants. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, , 1-22.	3.5	4
3	Understanding the Electronic Structure and Optical Properties of Vacancy-Ordered Double Perovskite A ₂ BX ₆ for Optoelectronic Applications. <i>Energy & Fuels</i> , 2022, 36, 7065-7074.	5.1	18
4	Proton-Coupled Electron Transfer in the Aqueous Nanochannels of Lyotropic Liquid Crystals: Interplay of H-Bonding and Polarity Effects. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 2651-2659.	4.6	6
5	Emergence of Aggregation Induced Emission (AIE), Room-Temperature Phosphorescence (RTP), and Multistimuli Response from a Single Organic Luminogen by Directed Structural Modification. <i>Journal of Physical Chemistry B</i> , 2021, 125, 12832-12846.	2.6	6
6	Inhibition Ability of Natural Compounds on Receptor-Binding Domain of SARS-CoV2: An In Silico Approach. <i>Pharmaceuticals</i> , 2021, 14, 1328.	3.8	10
7	Peculiar hydrogen bonding behaviour of water molecules inside the aqueous nanochannels of lyotropic liquid crystals. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 6210-6221.	2.8	3
8	Descriptors to Predict Dye-Sensitized Semiconductor Based Photocatalyst for Hydrogen Evolution Reaction. <i>ChemCatChem</i> , 2019, 11, 6460-6466.	3.7	1
9	Structural characteristics requisite for the ligand-based selective detection of i-motif DNA. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 5392-5399.	2.8	12
10	Sensitizing with short conjugated molecules: Multimodal anchoring on ZnO nanoparticles for enhanced electron transfer characteristics, stability and H ₂ evolution. <i>Catalysis Today</i> , 2018, 309, 89-97.	4.4	7
11	Spectroscopy and Dynamics of Cryptolepine in the Nanocavity of Cucurbit[7]uril and DNA. <i>ChemPhysChem</i> , 2016, 17, 506-515.	2.1	15
12	Nuclear quantum effects in a HIV/cancer inhibitor: The case of ellipticine. <i>Journal of Chemical Physics</i> , 2016, 145, 205102.	3.0	24
13	Coordination polymers of Fe(III) and Al(III) ions with TCA ligand: distinctive fluorescence, CO ₂ uptake, redox-activity and oxygen evolution reaction. <i>Dalton Transactions</i> , 2016, 45, 6901-6908.	3.3	17
14	Surface Site Modulations by Conjugated Organic Molecules To Enhance Visible Light Activity of ZnO Nanostructures in Photocatalytic Water Splitting. <i>Journal of Physical Chemistry C</i> , 2015, 119, 3060-3067.	3.1	24
15	Synthesis of Thermally Stable Energetic 1,2,3-Triazole Derivatives. <i>Chemistry - A European Journal</i> , 2013, 19, 509-518.	3.3	58