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List of Publications by Year
in descending order

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11 papers	155 citations	1478505 6 h-index	1281871 11 g-index
11 all docs	11 docs citations	11 times ranked	143 citing authors

#	Article	IF	Citations
1	Novel Xanthate Complexes for the Size-Controlled Synthesis of Copper Sulfide Nanorods. Inorganic Chemistry, 2017, 56, 9247-9254.	4.0	39
2	Tuning optoelectronic properties of triphenylamine based dyes through variation of pi-conjugated units and anchoring groups: A DFT/TD-DFT investigation. Journal of Molecular Graphics and Modelling, 2020, 94, 107480.	2.4	31
3	Effects of heteroatoms in Ï€-conjugated linkers on the optical and electronic properties of modified triphenylamine based dyes: towards DSSCsâ€™ applications. Journal of Molecular Modeling, 2020, 26, 288.	1.8	23
4	Luteolin: a blocker of SARS-CoV-2 cell entry based on relaxed complex scheme, molecular dynamics simulation, and metadynamics. Journal of Molecular Modeling, 2021, 27, 221.	1.8	17
5	Investigation of optoelectronic properties of triphenylamine-based dyes featuring heterocyclic anchoring groups for DSSCsâ€™ applications: a theoretical study. Structural Chemistry, 2020, 31, 2451-2461.	2.0	13
6	Influence of heteroatoms on the optoelectronic properties of triphenylamine-based dyes for DSSCs application: A computational approach. Computational and Theoretical Chemistry, 2022, 1210, 113644.	2.5	8
7	Ensemble-based screening of natural products and FDA-approved drugs identified potent inhibitors of SARS-CoV-2 that work with two distinct mechanisms. Journal of Molecular Graphics and Modelling, 2021, 105, 107871.	2.4	7
8	Effect of substituent in the acceptor on optical and electronic properties of triphenylamine based dyes: A density functional theory/time-dependent density functional theory investigation. Materials Science in Semiconductor Processing, 2022, 150, 106935.	4.0	7
9	Hydrophobic Ï€-Ï€ stacking interactions and hydrogen bonds drive self-aggregation of luteolin in water. Journal of Molecular Graphics and Modelling, 2022, 116, 108243.	2.4	6
10	Optical and electronic properties of para-functionalized triphenylamine-based dyes: a theoretical study. Structural Chemistry, 2022, 33, 409-419.	2.0	2
11	A Molecular Investigation of the Solvent Influence on Inter- and Intra-Molecular Hydrogen Bond Interaction of Linamarin. Processes, 2022, 10, 352.	2.8	2