

Viki Kumar Prasad

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	Molecular Engineering of Triphenylamine Based Aggregation Enhanced Emissive Fluorophore: Structure-Dependent Mechanochromism and Self-Reversible Fluorescence Switching. <i>Crystal Growth and Design</i> , 2017, 17, 146-155.	1.4	75
2	BH9, a New Comprehensive Benchmark Data Set for Barrier Heights and Reaction Energies: Assessment of Density Functional Approximations and Basis Set Incompleteness Potentials. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 151-166.	2.3	27
3	Hydrogen Atom Transfer (HAT) Processes Promoted by the Quinolinimide- <i>N</i> -oxyl Radical. A Kinetic and Theoretical Study. <i>Journal of Organic Chemistry</i> , 2017, 82, 6133-6141.	1.7	25
4	PEPCONF, a diverse data set of peptide conformational energies. <i>Scientific Data</i> , 2019, 6, 180310.	2.4	23
5	Atom-Centered Potentials with Dispersion-Corrected Minimal-Basis-Set Hartree-Fock: An Efficient and Accurate Computational Approach for Large Molecular Systems. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 726-738.	2.3	18
6	BSE49, a diverse, high-quality benchmark dataset of separation energies of chemical bonds. <i>Scientific Data</i> , 2021, 8, 300.	2.4	9
7	Fast and Accurate Quantum Mechanical Modeling of Large Molecular Systems Using Small Basis Set Hartree-Fock Methods Corrected with Atom-Centered Potentials. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 2208-2232.	2.3	7
8	Performance of small basis set Hartree-Fock methods for modeling non-covalent interactions. <i>Electronic Structure</i> , 2021, 3, 034007.	1.0	6
9	Small-Basis Set Density-Functional Theory Methods Corrected with Atom-Centered Potentials. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 2913-2930.	2.3	4