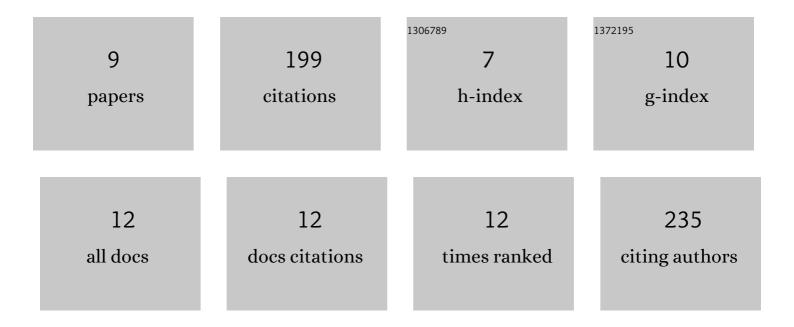
Viki Kumar Prasad

List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/7651466/publications.pdf Version: 2024-02-01



#	Article	IF	CITATIONS
1	Molecular Engineering of Triphenylamine Based Aggregation Enhanced Emissive Fluorophore: Structure-Dependent Mechanochromism and Self-Reversible Fluorescence Switching. Crystal Growth and Design, 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. Journal of Chemical Theory and Computation, 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. Journal of Organic Chemistry, 2017, 82, 6133-6141.	1.7	25
4	PEPCONF, a diverse data set of peptide conformational energies. Scientific Data, 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. Journal of Chemical Theory and Computation, 2018, 14, 726-738.	2.3	18
6	BSE49, a diverse, high-quality benchmark dataset of separation energies of chemical bonds. Scientific Data, 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. Journal of Chemical Theory and Computation, 2022, 18, 2208-2232.	2.3	7
8	Performance of small basis set Hartree–Fock methods for modeling non-covalent interactions. Electronic Structure, 2021, 3, 034007.	1.0	6
9	Small-Basis Set Density-Functional Theory Methods Corrected with Atom-Centered Potentials. Journal of Chemical Theory and Computation, 2022, 18, 2913-2930.	2.3	4