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List of Publications by Year in descending order

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Version: 2024-02-01

11
papers

682
citations

1039880

9
h-index

1281743

11
g-index

13
all docs

13
docs citations

13
times ranked

691
citing authors

#	ARTICLE	IF	CITATIONS
1	P<sc>SI4</sc> 1.4: Open-source software for high-throughput quantum chemistry. Journal of Chemical Physics, 2020, 152, 184108.	1.2	440
2	P<sc>si</sc>4N<sc>um</sc>P<sc>y</sc>: An Interactive Quantum Chemistry Programming Environment for Reference Implementations and Rapid Development. Journal of Chemical Theory and Computation, 2018, 14, 3504-3511.	2.3	106
3	Assessment of Density Functional Methods for Geometry Optimization of Bimolecular van der Waals Complexes. Journal of Chemical Theory and Computation, 2018, 14, 3004-3013.	2.3	27
4	Python implementation of the restrained electrostatic potential charge model. International Journal of Quantum Chemistry, 2020, 120, e26035.	1.0	17
5	Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCE<sc>ngine</sc>): Automation and interoperability among computational chemistry programs. Journal of Chemical Physics, 2021, 155, 204801.	1.2	15
6	Noncovalent Helicene Structure between Nucleic Acids and Cyanuric Acid. Chemistry - A European Journal, 2021, 27, 4043-4052.	1.7	14
7	X-ray Fiber Diffraction and Computational Analyses of Stacked Hexads in Supramolecular Polymers: Insight into Self-Assembly in Water by Prospective Prebiotic Nucleobases. Journal of the American Chemical Society, 2021, 143, 6079-6094.	6.6	13
8	Solvent, temperature and concentration effects on the optical rotatory dispersion of (R)-3-methylcyclohexanone. Journal of Molecular Structure, 2017, 1130, 19-25.	1.8	12
9	The proto-Nucleic Acid Builder: a software tool for constructing nucleic acid analogs. Nucleic Acids Research, 2021, 49, 79-89.	6.5	10
10	Tuning DNA Supramolecular Polymers by the Addition of Small, Functionalized Nucleobase Mimics. Journal of the American Chemical Society, 2021, 143, 19824-19833.	6.6	10
11	Density functional theory study of the substituent effect on the structure, conformation and vibrational spectra in halosubstituted anilines. RSC Advances, 2016, 6, 67794-67804.	1.7	6