Thomas Weymuth

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/1006435/publications.pdf

Version: 2024-02-01

18	517	840585 11	940416 16
papers	citations	h-index	g-index

20	20	20	748
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	New Benchmark Set of Transition-Metal Coordination Reactions for the Assessment of Density Functionals. Journal of Chemical Theory and Computation, 2014, 10, 3092-3103.	2.3	181
2	M<scp>O</scp>V<scp>I</scp>P<scp>AC</scp>: Vibrational spectroscopy with a robust metaâ€program for massively parallel standard and inverse calculations. Journal of Computational Chemistry, 2012, 33, 2186-2198.	1.5	59
3	A Local-Mode Model for Understanding the Dependence of the Extended Amide III Vibrations on Protein Secondary Structure. Journal of Physical Chemistry B, 2010, 114, 10649-10660.	1.2	55
4	Inverse quantum chemistry: Concepts and strategies for rational compound design. International Journal of Quantum Chemistry, 2014, 114, 823-837.	1.0	47
5	Gradientâ€driven molecule construction: An inverse approach applied to the design of smallâ€molecule fixating catalysts. International Journal of Quantum Chemistry, 2014, 114, 838-850.	1.0	27
6	Statistical Analysis of Semiclassical Dispersion Corrections. Journal of Chemical Theory and Computation, 2018, 14, 2480-2494.	2.3	25
7	Characteristic Raman Optical Activity Signatures of Protein Î²-Sheets. Journal of Physical Chemistry B, 2013, 117, 11943-11953.	1.2	24
8	Redoxâ€Active Chiroptical Switching in Monoâ€and Bisâ€iron Ethynylcarbo[6]helicenes Studied by Electronic and Vibrational Circular Dichroism and Resonance Raman Optical Activity. Chemistry - A European Journal, 2018, 24, 15067-15079.	1.7	24
9	How Many Chiral Centers Can Raman Optical Activity Spectroscopy Distinguish in a Molecule?. Journal of Physical Chemistry A, 2012, 116, 5410-5419.	1.1	16
10	Expansive Quantum Mechanical Exploration of Chemical Reaction Paths. Accounts of Chemical Research, 2022, 55, 35-43.	7.6	14
11	Identifying Protein Î²-Turns with Vibrational Raman Optical Activity. ChemPhysChem, 2011, 12, 1165-1175.	1.0	13
12	Immersive Interactive Quantum Mechanics for Teaching and Learning Chemistry. Chimia, 2021, 75, 45.	0.3	8
13	The transferability limits of static benchmarks. Physical Chemistry Chemical Physics, 2022, 24, 14692-14698.	1.3	8
14	Systematic dependence of transitionâ€metal coordination energies on densityâ€functional parametrizations. International Journal of Quantum Chemistry, 2015, 115, 90-98.	1.0	6
15	Toward an Inverse Approach for the Design of Small-Molecule Fixating Catalysts. Materials Research Society Symposia Proceedings, 2013, 1524, 101.	0.1	5
16	Ultraâ€fast spectroscopy for <scp>highâ€throughput</scp> and interactive quantum chemistry. International Journal of Quantum Chemistry, 0, , .	1.0	2
17	Resonance Effects in the Raman Optical Activity Spectrum of [Rh(en)₃]³⁺. Journal of Physical Chemistry A, 2019, 123, 9357-9370.	1.1	1
18	Heuristics and Uncertainty Quantification in Rational and Inverse Compound and Catalyst Design. , 2024, , 485-495.		0