

Thomas Weymuth

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

17
papers

409
citations

10
h-index

20
g-index

20
ext. papers

468
ext. citations

4.5
avg, IF

3.89
L-index

#	Paper	IF	Citations
17	Expansive Quantum Mechanical Exploration of Chemical Reaction Paths.. <i>Accounts of Chemical Research</i> , 2021 ,	24.3	5
16	Immersive Interactive Quantum Mechanics for Teaching and Learning Chemistry. <i>Chimia</i> , 2021 , 75, 45-49	1.3	5
15	Resonance Effects in the Raman Optical Activity Spectrum of [Rh(en)]. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 9357-9370	2.8	1
14	Statistical Analysis of Semiclassical Dispersion Corrections. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 2480-2494	6.4	18
13	Redox-Active Chiroptical Switching in Mono- and Bis-Iron Ethynylcarbo[6]helicenes Studied by Electronic and Vibrational Circular Dichroism and Resonance Raman Optical Activity. <i>Chemistry - A European Journal</i> , 2018 , 24, 15067-15079	4.8	19
12	Systematic dependence of transition-metal coordination energies on density-functional parametrizations. <i>International Journal of Quantum Chemistry</i> , 2015 , 115, 90-98	2.1	6
11	Inverse quantum chemistry: Concepts and strategies for rational compound design. <i>International Journal of Quantum Chemistry</i> , 2014 , 114, 823-837	2.1	42
10	New Benchmark Set of Transition-Metal Coordination Reactions for the Assessment of Density Functionals. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 3092-103	6.4	142
9	Gradient-driven molecule construction: An inverse approach applied to the design of small-molecule fixating catalysts. <i>International Journal of Quantum Chemistry</i> , 2014 , 114, 838-850	2.1	24
8	Characteristic Raman optical activity signatures of protein β sheets. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 11943-53	3.4	23
7	Toward an Inverse Approach for the Design of Small-Molecule Fixating Catalysts. <i>Materials Research Society Symposia Proceedings</i> , 2013 , 1524, 101		4
6	How many chiral centers can Raman optical activity spectroscopy distinguish in a molecule?. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 5410-9	2.8	10
5	M(O)V(I)P(AC): vibrational spectroscopy with a robust meta-program for massively parallel standard and inverse calculations. <i>Journal of Computational Chemistry</i> , 2012 , 33, 2186-98	3.5	50
4	Density Functional Theory for Transition Metal Chemistry: The Case of a Water-Splitting Ruthenium Cluster 2011 , 137-163		2
3	Identifying protein β turns with vibrational Raman optical activity. <i>ChemPhysChem</i> , 2011 , 12, 1165-75	3.2	13
2	A local-mode model for understanding the dependence of the extended amide III vibrations on protein secondary structure. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 10649-60	3.4	44
1	The Transferability Limits of Static Benchmarks. <i>Physical Chemistry Chemical Physics</i> ,	3.6	1

