

Thomas R Furlani

List of Publications by Year in descending order

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11
papers

6,729
citations

840119

11
h-index

1281420

11
g-index

11
all docs

11
docs citations

11
times ranked

7267
citing authors

#	ARTICLE	IF	CITATIONS
1	Advances in methods and algorithms in a modern quantum chemistry program package. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 3172-3191.	1.3	2,597
2	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. <i>Molecular Physics</i> , 2015, 113, 184-215.	0.8	2,561
3	Q-Chem 2.0: a high-performance ab initio electronic structure program package. <i>Journal of Computational Chemistry</i> , 2000, 21, 1532-1548.	1.5	617
4	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , 2021, 155, 084801.	1.2	518
5	Theory of spin-orbit coupling. Application to singlet-triplet interaction in the trimethylene biradical. <i>Journal of Chemical Physics</i> , 1985, 82, 5577-5583.	1.2	117
6	Combined X-ray Diffraction and Density Functional Study of [Ni(NO)(η^5 -Cp*)] in the Ground and Light-Induced Metastable States. <i>Inorganic Chemistry</i> , 1998, 37, 1519-1526.	1.9	87
7	Hydrophobic and Hydrogen-Bonding Effects on the Rate of Diels-Alder Reactions in Aqueous Solution. <i>Journal of Organic Chemistry</i> , 1996, 61, 5492-5497.	1.7	83
8	Computation of one and two electron spin-orbit integrals. <i>Journal of Computational Chemistry</i> , 1988, 9, 771-778.	1.5	67
9	Efficient computation of the dispersion interaction with density-functional theory. <i>Physical Review A</i> , 2009, 79, .	1.0	53
10	Metastable Decomposition of {ROH} _n H ⁺ Cluster Ions (Where R = CH ₃ or CH ₃ CH ₂). <i>The Journal of Physical Chemistry</i> , 1996, 100, 12235-12240.	2.9	15
11	Transition states for H atom transfer reactions in the CH ₂ CH ₂ OH radical: The effect of a water molecule. <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 5063.	1.3	14