Thomas R Furlani

List of Publications by Year
in descending order

11 papers	6,729 citations	840776 11 h-index	1281871 11 g-index
11 all docs	11 docs citations	11 times ranked	7267 citing authors

#	Article	IF	Citations
1	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	3.0	518
2	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,561
3	Efficient computation of the dispersion interaction with density-functional theory. Physical Review A, 2009, 79, .	2.5	53
4	Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191.	2.8	2,597
5	Transition states for H atom transfer reactions in the CH2CH2OH radical: The effect of a water molecule. Physical Chemistry Chemical Physics, 2003, 5, 5063.	2.8	14
6	Q-Chem 2.0: a high-performanceab initio electronic structure program package. Journal of Computational Chemistry, 2000, 21, 1532-1548.	3.3	617
7	Combined X-ray Diffraction and Density Functional Study of [Ni(NO)(Î·5-Cp*)] in the Ground and Light-Induced Metastable States. Inorganic Chemistry, 1998, 37, 1519-1526.	4.0	87
8	Hydrophobic and Hydrogen-Bonding Effects on the Rate of Dielsâ^'Alder Reactions in Aqueous Solution. Journal of Organic Chemistry, 1996, 61, 5492-5497.	3.2	83
9	Metastable Decomposition of {ROH}nH+ Cluster Ions (Where R = CH3 or CH3CH2). The Journal of Physical Chemistry, 1996, 100, 12235-12240.	2.9	15
10	Computation of one and two electron spin-orbit integrals. Journal of Computational Chemistry, 1988, 9, 771-778.	3.3	67
11	Theory of spinâ€orbit coupling. Application to singletâ€“triplet interaction in the trimethylene biradical. Journal of Chemical Physics, 1985, 82, 5577-5583.	3.0	117