William C Isley Iii

List of Publications by Year
in descending order

13	1,268	840585	1125617
papers	citations	11 h-index	13 g-index

13	13	13	2534
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Destruction of chemical warfare agents using metalâ€“organic frameworks. Nature Materials, 2015, 14, 512-516.	13.3	790
2	Design of a Metalâ€“Organic Framework with Enhanced Back Bonding for Separation of N₂ and CH₄. Journal of the American Chemical Society, 2014, 136, 698-704.	6.6	157
3	Proof for the Concerted Inversion Mechanism in the transâ†'cis Isomerization of Azobenzene Using Hydrogen Bonding To Induce Isomer Locking. Journal of Organic Chemistry, 2010, 75, 4817-4827.	1.7	79
4	Empirical and Theoretical Insights into the Structural Features and Hostâ€“Guest Chemistry of M₈L₄ Tube Architectures. Journal of the American Chemical Society, 2014, 136, 3972-3980.	6.6	40
5	Electrochemical Reduction of 2,4-Dinitrotoluene in Aprotic and pH-Buffered Media. Journal of Physical Chemistry C, 2015, 119, 13088-13097.	1.5	33
6	Predicting paramagnetic ¹H NMR chemical shifts and state-energy separations in spin-crossover hostâ€“guest systems. Physical Chemistry Chemical Physics, 2014, 16, 10620-10628.	1.3	32
7	Ab Initio Extension of the AMOEBA Polarizable Force Field to Fe²⁺. Journal of Chemical Theory and Computation, 2013, 9, 3062-3071.	2.3	31
8	Quantum Chemical Methods for Modeling Covalent Modification of Biological Thiols. Journal of Computational Chemistry, 2020, 41, 427-438.	1.5	31
9	Optimization and prediction of the electronâ€“nuclear dipolar and scalar interaction in¹H and¹³C liquid state dynamic nuclear polarization. Chemical Science, 2015, 6, 6482-6495.	3.7	27
10	Prediction of ¹⁹F NMR Chemical Shifts in Labeled Proteins: Computational Protocol and Case Study. Molecular Pharmaceutics, 2016, 13, 2376-2386.	2.3	23
11	Molecular Modeling Characterization of a Conformationally Constrained Monolayer-Protected Gold Cluster. Journal of Physical Chemistry C, 2010, 114, 16043-16050.	1.5	11
12	In situ microscopy across scales for the characterization of crystal growth mechanisms: the case of europium oxalate. CrystEngComm, 2018, 20, 2822-2833.	1.3	10
13	Electric Potentials of Metastable Salt Clusters. Journal of Physical Chemistry C, 2019, 123, 14010-14023.	1.5	4