William C Isley Iii

List of Publications by Year in Descending Order

13 papers	1,035 citations	11 h-index	13 g-index
13 ext. papers	1,166 ext. citations	8 avg, IF	3.54 L-index

#	Paper	IF	Citations
13	Quantum Chemical Methods for Modeling Covalent Modification of Biological Thiols. *Journal of Computational Chemistry*, **2020**, 41, 427-438	3.5	18
12	Electric Potentials of Metastable Salt Clusters. *Journal of Physical Chemistry C*, **2019**, 123, 14010-14023	3.8	3
11	In situ microscopy across scales for the characterization of crystal growth mechanisms: the case of europium oxalate. *CrystEngComm*, **2018**, 20, 2822-2833	3.3	3
10	Prediction of (19)F NMR Chemical Shifts in Labeled Proteins: Computational Protocol and Case Study. *Molecular Pharmaceutics*, **2016**, 13, 2376-86	5.6	18
9	Destruction of chemical warfare agents using metal-organic frameworks. *Nature Materials*, **2015**, 14, 512-6	27	647
8	Electrochemical Reduction of 2,4-Dinitrotoluene in Aprotic and pH-Buffered Media. *Journal of Physical Chemistry C*, **2015**, 119, 13088-13097	3.8	25
7	Optimization and prediction of the electron-nuclear dipolar and scalar interaction in H and C liquid state dynamic nuclear polarization. *Chemical Science*, **2015**, 6, 6482-6495	9.4	21
6	Design of a metal-organic framework with enhanced back bonding for separation of N□and CH□ *Journal of the American Chemical Society*, **2014**, 136, 698-704	16.4	134
5	Predicting paramagnetic 1H NMR chemical shifts and state-energy separations in spin-crossover host-guest systems. *Physical Chemistry Chemical Physics*, **2014**, 16, 10620-8	3.6	31
4	Empirical and theoretical insights into the structural features and host-guest chemistry of M8L4 tube architectures. *Journal of the American Chemical Society*, **2014**, 136, 3972-80	16.4	28
3	Ab Initio Extension of the AMOEBA Polarizable Force Field to Fe(2.). *Journal of Chemical Theory and Computation*, **2013**, 9, 3062-71	6.4	26
2	Molecular Modeling Characterization of a Conformationally Constrained Monolayer-Protected Gold Cluster□*Journal of Physical Chemistry C*, **2010**, 114, 16043-16050	3.8	11
1	Proof for the concerted inversion mechanism in the trans-->cis isomerization of azobenzene using hydrogen bonding to induce isomer locking. *Journal of Organic Chemistry*, **2010**, 75, 4817-27	4.2	70