James L Mcdonagh

List of Publications by Year
in descending order

15 papers	405 citations	840776 11 h-index	1058476 14 g-index
19 all docs	19 docs citations	19 times ranked	454 citing authors

#	Article	IF	Citations
1	First-Principles Calculation of the Intrinsic Aqueous Solubility of Crystalline Druglike Molecules. Journal of Chemical Theory and Computation, 2012, 8, 3322-3337.	5.3	84
2	Uniting Cheminformatics and Chemical Theory To Predict the Intrinsic Aqueous Solubility of Crystalline Druglike Molecules. Journal of Chemical Information and Modeling, 2014, 54, 844-856.	5.4	68
3	Quantifying Electron Correlation of the Chemical Bond. Journal of Physical Chemistry Letters, 2017, 8, 1937-1942.	4.6	41
4	Utilizing Machine Learning for Efficient Parameterization of Coarse Grained Molecular Force Fields. Journal of Chemical Information and Modeling, 2019, 59, 4278-4288.	5.4	36
5	Partitioning dynamic electron correlation energy: Viewing Møller-Plesset correlation energies through Interacting Quantum Atom (IQA) energy partitioning. Chemical Physics Letters, 2016, 662, 228-234.	2.6	33
6	Machine Learning of Dynamic Electron Correlation Energies from Topological Atoms. Journal of Chemical Theory and Computation, 2018, 14, 216-224.	5.3	29
7	Are the Sublimation Thermodynamics of Organic Molecules Predictable?. Journal of Chemical Information and Modeling, 2016, 56, 2162-2179.	5.4	28
8	Challenge to Reconcile Experimental Micellar Properties of the CnEm Nonionic Surfactant Family. Journal of Physical Chemistry B, 2019, 123, 1696-1707.	2.6	22
9	Enzyme Informatics. Current Topics in Medicinal Chemistry, 2012, 12, 1911-1923.	2.1	20
10	The Transferability of Topologically Partitioned Electron Correlation Energies in Water Clusters. ChemPhysChem, 2017, 18, 3360-3368.	2.1	13
11	The effects of higher orders of perturbation theory on the correlation energy of atoms and bonds in molecules. International Journal of Quantum Chemistry, 2018, 118, e25519.	2.0	13
12	What can digitisation do for formulated product innovation and development?. Polymer International, 2021, 70, 248-255.	3.1	10
13	University-level practical activities in bioinformatics benefit voluntary groups of pupils in the last 2Âyears of school. International Journal of STEM Education, 2015, 2, .	5.0	5
14	Bringing computational science to the public. SpringerPlus, 2016, 5, 259.	1.2	2
15	3. In Silico methods to predict solubility. , 2019, , 71-112.		1