James L Mcdonagh

List of Publications by Year
in descending order

15	405	949033 11	1181555 14
papers	citations	h-index	g-index

19	19	19	507
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	What can digitisation do for formulated product innovation and development?. Polymer International, 2021, 70, 248-255.	1.6	10
2	Utilizing Machine Learning for Efficient Parameterization of Coarse Grained Molecular Force Fields. Journal of Chemical Information and Modeling, 2019, 59, 4278-4288.	2.5	36
3	Challenge to Reconcile Experimental Micellar Properties of the CnEm Nonionic Surfactant Family. Journal of Physical Chemistry B, 2019, 123, 1696-1707.	1.2	22
4	3. In Silico methods to predict solubility. , 2019, , 71-112.		1
5	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.	1.0	13
6	Machine Learning of Dynamic Electron Correlation Energies from Topological Atoms. Journal of Chemical Theory and Computation, 2018, 14, 216-224.	2.3	29
7	Quantifying Electron Correlation of the Chemical Bond. Journal of Physical Chemistry Letters, 2017, 8, 1937-1942.	2.1	41
8	The Transferability of Topologically Partitioned Electron Correlation Energies in Water Clusters. ChemPhysChem, 2017, 18, 3360-3368.	1.0	13
9	Bringing computational science to the public. SpringerPlus, 2016, 5, 259.	1.2	2
10	Partitioning dynamic electron correlation energy: Viewing MÃ¸ller-Plesset correlation energies through Interacting Quantum Atom (IQA) energy partitioning. Chemical Physics Letters, 2016, 662, 228-234.	1.2	33
11	Are the Sublimation Thermodynamics of Organic Molecules Predictable?. Journal of Chemical Information and Modeling, 2016, 56, 2162-2179.	2.5	28
12	University-level practical activities in bioinformatics benefit voluntary groups of pupils in the last 2Âyears of school. International Journal of STEM Education, 2015, 2, .	2.7	5
13	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.	2.5	68
14	Enzyme Informatics. Current Topics in Medicinal Chemistry, 2012, 12, 1911-1923.	1.0	20
15	First-Principles Calculation of the Intrinsic Aqueous Solubility of Crystalline Druglike Molecules. Journal of Chemical Theory and Computation, 2012, 8, 3322-3337.	2.3	84