Mark P Waller

List of Publications by Year
in descending order

42 papers	3,984 citations	331670 21 h-index	265206 42 g-index
44 all docs	44 docs citations	44 times ranked	4774 citing authors

#	Article	IF	Citations
1	Planning chemical syntheses with deep neural networks and symbolic AI. Nature, 2018, 555, 604-610.	27.8	1,122
2	Generating Focused Molecule Libraries for Drug Discovery with Recurrent Neural Networks. ACS Central Science, 2018, 4, 120-131.	11.3	908
3	Neuralâ€Symbolic Machine Learning for Retrosynthesis and Reaction Prediction. Chemistry - A European Journal, 2017, 23, 5966-5971.	3.3	334
4	Hybrid density functional theory for Ï€-stacking interactions: Application to benzenes, pyridines, and DNA bases. Journal of Computational Chemistry, 2006, 27, 491-504.	3.3	236
5	Geometries of Second-Row Transition-Metal Complexes from Density-Functional Theory. Journal of Chemical Theory and Computation, 2007, 3, 2234-2242.	5.3	154
6	Modelling Chemical Reasoning to Predict and Invent Reactions. Chemistry - A European Journal, 2017, 23, 6118-6128.	3.3	142
7	Cholesterol Effect on the Dipole Potential of Lipid Membranes. Biophysical Journal, 2006, 90, 4060-4070.	0.5	134
8	51Vâ€...NMR Chemical Shifts Calculated from QM/MM Models of Vanadium Chloroperoxidase. Chemistry - A European Journal, 2007, 13, 4723-4732.	3.3	95
9	A QM/MM refinement of an experimental DNA structure with metal-mediated base pairs. Journal of Inorganic Biochemistry, 2013, 127, 203-210.	3.5	67
10	Investigating inclusion complexes using quantum chemical methods. Chemical Society Reviews, 2012, 41, 3119.	38.1	60
11	51V NMR Chemical Shifts Calculated from QM/MM Models of Peroxo Forms of Vanadium Haloperoxidases. Journal of Physical Chemistry B, 2009, 113, 4456-4465.	2.6	52
12	Adaptive quantum mechanics/molecular mechanics methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 369-385.	14.6	51
13	A Densityâ€Based Adaptive Quantum Mechanical/Molecular Mechanical Method. ChemPhysChem, 2014, 15, 3218-3225.	2.1	50
14	Experimental and Theoretical Charge Density Studies of Tetrafluorophthalonitrile and Tetrafluoroisophthalonitrile. Journal of Physical Chemistry B, 2004, 108, 3663-3672.	2.6	48
15	Peptideâ€Based Carbohydrate Receptors. Chemistry - A European Journal, 2014, 20, 2770-2782.	3.3	41
16	ChemPreview : an augmented reality-based molecular interface. Journal of Molecular Graphics and Modelling, 2017, 73, 18-23.	2.4	41
17	51V NMR Chemical Shifts from Quantum-Mechanical/Molecular-Mechanical Models of Vanadium Bromoperoxidase. Journal of Physical Chemistry B, 2008, 112, 5813-5823.	2.6	39
18	pH response and molecular recognition in a low molecular weight peptide hydrogel. Organic and Biomolecular Chemistry, 2015, 13, 561-569.	2.8	36

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19	Sequenceâ€Dependent Duplex Stabilization upon Formation of a Metalâ€Mediated Base Pair. Chemistry - A European Journal, 2016, 22, 295-301.	3.3	29
20	Vibrational corrections to geometries of transition metal complexes from density functional theory. Journal of Computational Chemistry, 2007, 28, 1531-1537.	3.3	27
21	Q | R: quantum-based refinement. Acta Crystallographica Section D: Structural Biology, 2017, 73, 45-52.	2.3	24
22	A new orbital-based model for the analysis of experimental molecular charge densities: an application to (Z)-N-methyl-C-phenylnitrone. Physical Chemistry Chemical Physics, 2005, 7, 1772.	2.8	23
23	The Presumption of Innocence? A DFT-Directed Verdict on Oxidized Amavadin and Vanadium Catecholate Complexes. Inorganic Chemistry, 2007, 46, 11297-11307.	4.0	21
24	Experimental and theoretical charge distribution in (Z)-N-methyl-C-phenylnitrone. Organic and Biomolecular Chemistry, 2003, 1, 1034-1040.	2.8	20
25	Solving the scalability issue in quantum-based refinement: Q|R#1. Acta Crystallographica Section D: Structural Biology, 2017, 73, 1020-1028.	2.3	20
26	Rational Density Functional Selection Using Game Theory. Journal of Chemical Information and Modeling, 2018, 58, 61-67.	5.4	20
27	Experimental and Theoretical Charge Density Distribution in Two Ternary Cobalt(III) Complexes of Aromatic Amino Acids. Journal of Physical Chemistry A, 2007, 111, 10123-10133.	2.5	19
28	A Systematic Approach to Identify Cooperatively Bound Homotrimers. Journal of Physical Chemistry A, 2013, 117, 174-182.	2.5	18
29	Revealing noncovalent interactions in quantum crystallography: Taurine revisited. Journal of Computational Chemistry, 2013, 34, 466-470.	3.3	17
30	Toward more efficient densityâ€based adaptive QM/MM methods. International Journal of Quantum Chemistry, 2017, 117, e25336.	2.0	17
31	Hybrid Metaheuristic Approach for Nonlocal Optimization of Molecular Systems. Journal of Chemical Theory and Computation, 2013, 9, 2137-2149.	5.3	16
32	Naturally and synthetically linked lys48 diubiquitin: a QM/MM study. RSC Advances, 2013, 3, 16122.	3.6	14
33	Flavone. Acta Crystallographica Section E: Structure Reports Online, 2003, 59, o767-o768.	0.2	13
34	Yoink: An interactionâ€based partitioning API. Journal of Computational Chemistry, 2018, 39, 799-806.	3.3	13
35	Including crystallographic symmetry in quantum-based refinement: Q | R#2. Acta Crystallographica Section D: Structural Biology, 2020, 76, 41-50.	2.3	13
36	Influence of Crystal Effects on Molecular Charge Densities in a Study of 9-Ethynyl-9-fluorenol. Journal of Physical Chemistry A, 2003, 107, 11201-11208.	2.5	12

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37	JACOB: An enterprise framework for computational chemistry. Journal of Computational Chemistry, 2013, 34, 1420-1428.	3.3	10
38	Real-space quantum-based refinement for cryo-EM: Q | R#3. Acta Crystallographica Section D: Structural Biology, 2020, 76, 1184-1191.	2.3	7
39	A Probabilistic Framework for Constructing Temporal Relations in Replica Exchange Molecular Trajectories. Journal of Chemical Theory and Computation, 2018, 14, 3365-3380.	5.3	6
40	Assessment of Weak Intermolecular Interactions Across QM/MM Noncovalent Boundaries. Journal of Chemical Information and Modeling, 2012, 52, 93-98.	5.4	5
41	Cooperativity in bimetallic glutathione complexes. Journal of Molecular Graphics and Modelling, 2015, 62, 1-10.	2.4	5
42	JACOB: A Dynamic Database for Computational Chemistry Benchmarking. Journal of Chemical Information and Modeling, 2012, 52, 3255-3262.	5.4	4