James J P Stewart

List of Publications by Citations

30 papers	28,323 citations	21 h-index	30 g-index
30 ext. papers	29,460 ext. citations	3.4 avg, IF	7.64 L-index

#	Paper	IF	Citations
30	Development and use of quantum mechanical molecular models. 76. AM1: a new general purpose quantum mechanical molecular model. *Journal of the American Chemical Society*, **1985**, 107, 3902-3909	16.4	12010
29	Optimization of parameters for semiempirical methods I. Method. *Journal of Computational Chemistry*, **1989**, 10, 209-220	3.5	6553
28	Optimization of parameters for semiempirical methods II. Applications. *Journal of Computational Chemistry*, **1989**, 10, 221-264	3.5	3335
27	Optimization of parameters for semiempirical methods V: modification of NDDO approximations and application to 70 elements. *Journal of Molecular Modeling*, **2007**, 13, 1173-213	2	2577
26	Optimization of parameters for semiempirical methods VI: more modifications to the NDDO approximations and re-optimization of parameters. *Journal of Molecular Modeling*, **2013**, 19, 1-32	2	1126
25	RM1: a reparameterization of AM1 for H, C, N, O, P, S, F, Cl, Br, and I. *Journal of Computational Chemistry*, **2006**, 27, 1101-11	3.5	571
24	Optimization of parameters for semiempirical methods. III Extension of PM3 to Be, Mg, Zn, Ga, Ge, As, Se, Cd, In, Sn, Sb, Te, Hg, Tl, Pb, and Bi. *Journal of Computational Chemistry*, **1991**, 12, 320-341	3.5	553
23	Application of localized molecular orbitals to the solution of semiempirical self-consistent field equations. *International Journal of Quantum Chemistry*, **1996**, 58, 133-146	2.1	303
22	Location of transition states in reaction mechanisms. *Journal of the Chemical Society, Faraday Transactions 2*, **1984**, 80, 227		237
21	Application of the PM6 method to modeling proteins. *Journal of Molecular Modeling*, **2009**, 15, 765-805	2	235
20	Optimization of parameters for semiempirical methods IV: extension of MNDO, AM1, and PM3 to more main group elements. *Journal of Molecular Modeling*, **2004**, 10, 155-64	2	213
19	Application of the PM6 method to modeling the solid state. *Journal of Molecular Modeling*, **2008**, 14, 499-535	2	125
18	Comparison of the accuracy of semiempirical and some DFT methods for predicting heats of formation. *Journal of Molecular Modeling*, **2004**, 10, 6-12	2	95
17	Sparkle/PM7 Lanthanide Parameters for the Modeling of Complexes and Materials. *Journal of Chemical Theory and Computation*, **2013**, 9, 3333-3341	6.4	86
16	Insights into colour-tuning of chlorophyll optical response in green plants. *Physical Chemistry Chemical Physics*, **2015**, 17, 26599-606	3.6	37
15	A new rapid method for orbital localisation. *Journal of the Chemical Society, Faraday Transactions 2*, **1982**, 78, 285		35
14	Cluster model for solids. *Journal of the Chemical Society, Faraday Transactions 2*, **1980**, 76, 520		32

13	Use of Semiempirical Methods for Detecting Anomalies in Reported Enthalpies of Formation of Organic Compounds. *Journal of Physical and Chemical Reference Data*, **2004**, 33, 713-724	4.3	24
12	An investigation into the applicability of the semiempirical method PM7 for modeling the catalytic mechanism in the enzyme chymotrypsin. *Journal of Molecular Modeling*, **2017**, 23, 154	2	22
11	High-Throughput Calculations of Molecular Properties in the MedeA Environment: Accuracy of PM7 in Predicting Vibrational Frequencies, Ideal Gas Entropies, Heat Capacities, and Gibbs Free Energies of Organic Molecules. *Journal of Chemical & Engineering Data*, **2014**, 59, 3136-3143	2.8	21
10	X-Ray crystallographic and NMR evidence for a uniquely strong OH ? N hydrogen bond in the solid state and solution. *Journal of the Chemical Society Chemical Communications*, **1989**, 1722		21
9	Calculation of polymer elastic moduli using semiempirical methods. *International Journal of Quantum Chemistry*, **1986**, 30, 529-540	2.1	19
8	MNDO-Like Semiempirical Molecular Orbital Theory and Its Application to Large Systems **2011**, 259-286		18
7	An approach to creating a more realistic working model from a protein data bank entry. *Journal of Molecular Modeling*, **2015**, 21, 3	2	16
6	Accuracy issues involved in modeling in vivo protein structures using PM7. *Proteins: Structure, Function and Bioinformatics*, **2015**, 83, 1427-35	4.2	15
5	Self-consistent field convergence for proteins: a comparison of full and localized-molecular-orbital schemes. *Journal of Molecular Modeling*, **2014**, 20, 2159	2	12
4	A comparison of X-ray and calculated structures of the enzyme MTH1. *Journal of Molecular Modeling*, **2016**, 22, 168	2	10
3	A method for predicting individual residue contributions to enzyme specificity and binding-site energies, and its application to MTH1. *Journal of Molecular Modeling*, **2016**, 22, 259	2	8
2	An examination of the nature of localized molecular orbitals and their value in understanding various phenomena that occur in organic chemistry. *Journal of Molecular Modeling*, **2018**, 25, 7	2	8
1	Standards-based curation of a decade-old digital repository dataset of molecular information. *Journal of Cheminformatics*, **2015**, 7, 43	8.6	6