James J P Stewart

List of Publications by Year in descending order

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29 papers	32,140 citations	304368 22 h-index	476904 29 g-index
30 all docs	30 docs citations	30 times ranked	18412 citing authors

#	Article	IF	Citations
1	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.	6.6	13,340
2	Optimization of parameters for semiempirical methods I. Method. Journal of Computational Chemistry, 1989, 10, 209-220.	1.5	7,369
3	Optimization of parameters for semiempirical methods II. Applications. Journal of Computational Chemistry, 1989, 10, 221-264.	1.5	3,741
4	Optimization of parameters for semiempirical methods V: Modification of NDDO approximations and application to 70 elements. Journal of Molecular Modeling, 2007, 13, 1173-1213.	0.8	3,060
5	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.	0.8	1,508
6	RM1: A reparameterization of AM1 for H, C, N, O, P, S, F, Cl, Br, and I. Journal of Computational Chemistry, 2006, 27, 1101-1111.	1.5	634
7	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.	1.5	619
8	Application of localized molecular orbitals to the solution of semiempirical self-consistent field equations. International Journal of Quantum Chemistry, 1996, 58, 133-146.	1.0	350
9	Application of the PM6 method to modeling proteins. Journal of Molecular Modeling, 2009, 15, 765-805.	0.8	270
10	Location of transition states in reaction mechanisms. Journal of the Chemical Society, Faraday Transactions 2, 1984, 80, 227.	1.1	266
11	Optimization of parameters for semiempirical methods IV: extension of MNDO, AM1, and PM3 to more main group elements. Journal of Molecular Modeling, 2004, 10, 155-164.	0.8	253
12	Application of the PM6 method to modeling the solid state. Journal of Molecular Modeling, 2008, 14, 499-535.	0.8	148
13	Sparkle/PM7 Lanthanide Parameters for the Modeling of Complexes and Materials. Journal of Chemical Theory and Computation, 2013, 9, 3333-3341.	2.3	107
14	Comparison of the accuracy of semiempirical and some DFT methods for predicting heats of formation. Journal of Molecular Modeling, 2004, 10, 6-12.	0.8	104
15	Insights into colour-tuning of chlorophyll optical response in green plants. Physical Chemistry Chemical Physics, 2015, 17, 26599-26606.	1.3	46
16	A new rapid method for orbital localisation. Journal of the Chemical Society, Faraday Transactions 2, 1982, 78, 285.	1.1	41
17	Cluster model for solids. Journal of the Chemical Society, Faraday Transactions 2, 1980, 76, 520.	1.1	33
18	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.	0.8	30

#	Article	IF	Citations
19	Calculation of polymer elastic moduli using semiempirical methods. International Journal of Quantum Chemistry, 1986, 30, 529-540.	1.0	26
20	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.	1.0	26
21	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.	1.9	24
22	An approach to creating a more realistic working model from a protein data bank entry. Journal of Molecular Modeling, 2015, 21, 3.	0.8	24
23	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.	2.0	23
24	Accuracy issues involved in modeling in vivo protein structures using <scp>PM</scp> 7. Proteins: Structure, Function and Bioinformatics, 2015, 83, 1427-1435.	1.5	16
25	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, 2019, 25, 7.	0.8	16
26	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.	0.8	15
27	Self-consistent field convergence for proteins: a comparison of full and localized-molecular-orbital schemes. Journal of Molecular Modeling, 2014, 20, 2159.	0.8	12
28	A comparison of X-ray and calculated structures of the enzyme MTH1. Journal of Molecular Modeling, 2016, 22, 168.	0.8	11
29	Standards-based curation of a decade-old digital repository dataset of molecular information. Journal of Cheminformatics, 2015, 7, 43.	2.8	8