Robert W Molt

List of Publications by Year
in descending order

22 papers	345 citations	840776 11 h-index	839539 18 g-index
22 all docs	22 docs citations	22 times ranked	439 citing authors

#	Article	IF	Citations
1	Magnetic properties of stainless steels at room and cryogenic temperatures. Journal of Magnetism and Magnetic Materials, 2009, 321, 2107-2114.	2.3	46
2	â€œSkinnyâ€•and â€œFatâ€•DNA: Two New Double Helices. Journal of the American Chemical Society, 2018, 140, 11655-11660.	13.7	36
3	RDX Geometries, Excited States, and Revised Energy Ordering of Conformers via MP2 and CCSD(T) Methodologies: Insights into Decomposition Mechanism. Journal of Physical Chemistry A, 2011, 115, 884-890.	2.5	33
4	Metal Fluorides: Tools for Structural and Computational Analysis of Phosphoryl Transfer Enzymes. Topics in Current Chemistry, 2017, 375, 36.	5.8	29
5	Gas phase RDX decomposition pathways using coupled cluster theory. Physical Chemistry Chemical Physics, 2016, 18, 26069-26077.	2.8	27
6	¹⁹Fâ€…NMR and DFT Analysis Reveal Structural and Electronic Transition State Features for RhoAâ€Catalyzed GTP Hydrolysis. Angewandte Chemie - International Edition, 2016, 55, 3318-3322.	13.8	26
7	Singletâ€“triplet separations of di-radicals treated by the DEA/DIP-EOM-CCSD methods. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	24
8	Conformers of CL-20 Explosive and ab Initio Refinement Using Perturbation Theory: Implications to Detonation Mechanisms. Journal of Physical Chemistry A, 2012, 116, 12129-12135.	2.5	20
9	The Great Diversity of HMX Conformers: Probing the Potential Energy Surface Using CCSD(T). Journal of Physical Chemistry A, 2013, 117, 3467-3474.	2.5	14
10	Consecutive non-natural PZ nucleobase pairs in DNA impact helical structure as seen in 50 Î¼s molecular dynamics simulations. Nucleic Acids Research, 2017, 45, 3643-3653.	14.5	14
11	Facile C_{sp²}â€“C_{sp²} Bond Cleavage in Oxalic Acid-Derived Radicals. Journal of the American Chemical Society, 2015, 137, 3248-3252.	13.7	12
12	A GAPâ€GTPaseâ€GDPâ€Pi Intermediate Crystal Structure Analyzed by DFT Shows GTP Hydrolysis Involves Serial Proton Transfers. Chemistry - A European Journal, 2019, 25, 8484-8488.	3.3	11
13	Structure and Biophysics for a Six Letter DNA Alphabet that Includes Imidazo[1,2-a]-1,3,5-triazine-2(8H)-4(3H)-dione (X) and 2,4-Diaminopyrimidine (K). ACS Synthetic Biology, 2017, 6, 2118-2129.	3.8	10
14	Assessing the Influence of Mutation on GTPase Transition States by Using Xâ€ray Crystallography, ¹⁹Fâ€…NMR, and DFT Approaches. Angewandte Chemie - International Edition, 2017, 56, 9732-9735.	13.8	9
15	Tautomeric equilibria of isoguanine and related purine analogs. Nucleosides, Nucleotides and Nucleic Acids, 2017, 36, 256-274.	1.1	9
16	¹⁹Fâ€…NMR and DFT Analysis Reveal Structural and Electronic Transition State Features for RhoAâ€Catalyzed GTP Hydrolysis. Angewandte Chemie, 2016, 128, 3379-3383.	2.0	8
17	Molecular cluster perturbation theory. I. Formalism. Molecular Physics, 2015, 113, 3459-3470.	1.7	6
18	Singletâ€“triplet separations of di-radicals treated by the DEA/DIP-EOM-CCSD methods. Highlights in Theoretical Chemistry, 2016, , 153-165.	0.0	5

#	Article	IF	Citations
19	Octahedral Trifluoromagnesate, an Anomalous Metal Fluoride Species, Stabilizes the Transition State in a Biological Motor. ACS Catalysis, 2021, 11, 2769-2773.	11.2	4
20	Pragmatic ab initio prediction of enthalpies of formation for large molecules: accuracy of MP2 geometries and frequencies using CCSD(T) correlation energies. Journal of Molecular Modeling, 2013, 19, 2821-2824.	1.8	1
21	Assessing the Influence of Mutation on GTPase Transition States by Using Xâ€ray Crystallography, 19 Fâ€…NMR, and DFT Approaches. Angewandte Chemie, 2017, 129, 9864-9867.	2.0	1
22	Metal Fluorides: Tools for Structural and Computational Analysis of Phosphoryl Transfer Enzymes. Topics in Current Chemistry Collections, 2017, , 35-65.	0.5	0