

# Robert W Molt

## List of Publications by Year in descending order

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22  
papers

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citations

840776

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839539

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times ranked

439  
citing authors

#	ARTICLE	IF	CITATIONS
1	Octahedral Trifluoromagnesate, an Anomalous Metal Fluoride Species, Stabilizes the Transition State in a Biological Motor. ACS Catalysis, 2021, 11, 2769-2773.	11.2	4
2	A GAPâ€GTPaseâ€GDPâ€ <sup>i</sup> Intermediate Crystal Structure Analyzed by DFT Shows GTP Hydrolysis Involves Serial Proton Transfers. Chemistry - A European Journal, 2019, 25, 8484-8488.	3.3	11
3	â€Skinnyâ€and â€Fatâ€DNA: Two New Double Helices. Journal of the American Chemical Society, 2018, 140, 11655-11660.	13.7	36
4	Assessing the Influence of Mutation on GTPase Transition States by Using Xâ€ray Crystallography, <sup>19</sup> Fâ€NMR, and DFT Approaches. Angewandte Chemie - International Edition, 2017, 56, 9732-9735.	13.8	9
5	Consecutive non-natural PZ nucleobase pairs in DNA impact helical structure as seen in 50 <sup>1</sup> / <sub>4</sub> s molecular dynamics simulations. Nucleic Acids Research, 2017, 45, 3643-3653.	14.5	14
6	Assessing the Influence of Mutation on GTPase Transition States by Using Xâ€ray Crystallography, <sup>19</sup> Fâ€NMR, and DFT Approaches. Angewandte Chemie, 2017, 129, 9864-9867.	2.0	1
7	Metal Fluorides: Tools for Structural and Computational Analysis of Phosphoryl Transfer Enzymes. Topics in Current Chemistry, 2017, 375, 36.	5.8	29
8	Tautomeric equilibria of isoguanine and related purine analogs. Nucleosides, Nucleotides and Nucleic Acids, 2017, 36, 256-274.	1.1	9
9	Structure and Biophysics for a Six Letter DNA Alphabet that Includes Imidazo[1,2- <i>a</i> ]-1,3,5-triazine-2(8 <i>H</i> )-4(3 <i>H</i> )-dione (X) and 2,4-Diaminopyrimidine (K). ACS Synthetic Biology, 2017, 6, 2118-2129.	3.8	10
10	Metal Fluorides: Tools for Structural and Computational Analysis of Phosphoryl Transfer Enzymes. Topics in Current Chemistry Collections, 2017, , 35-65.	0.5	0
11	<sup>19</sup> Fâ€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
12	<sup>19</sup> Fâ€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
13	Gas phase RDX decomposition pathways using coupled cluster theory. Physical Chemistry Chemical Physics, 2016, 18, 26069-26077.	2.8	27
14	Singletâ€triplet separations of di-radicals treated by the DEA/DIP-EOM-CCSD methods. Highlights in Theoretical Chemistry, 2016, , 153-165.	0.0	5
15	Facile C <sup>sp2</sup> â€C <sup>sp2</sup> Bond Cleavage in Oxalic Acid-Derived Radicals. Journal of the American Chemical Society, 2015, 137, 3248-3252.	13.7	12
16	Molecular cluster perturbation theory. I. Formalism. Molecular Physics, 2015, 113, 3459-3470.	1.7	6
17	Singletâ€triplet separations of di-radicals treated by the DEA/DIP-EOM-CCSD methods. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	24
18	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

#	ARTICLE	IF	CITATIONS
19	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
20	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
21	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
22	Magnetic properties of stainless steels at room and cryogenic temperatures. Journal of Magnetism and Magnetic Materials, 2009, 321, 2107-2114.	2.3	46