Dmitry Ganyushin

List of Publications by Year
in descending order

13	1,477	687363 13	1125743 13
papers	citations	h-index	g-index

13	13	13	1618
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A fully variational spin-orbit coupled complete active space self-consistent field approach: Application to electron paramagnetic resonance g-tensors. Journal of Chemical Physics, 2013, 138, 104113.	3.0	106
2	Detailed Ab Initio First-Principles Study of the Magnetic Anisotropy in a Family of Trigonal Pyramidal Iron(II) Pyrrolide Complexes. Inorganic Chemistry, 2011, 50, 7460-7477.	4.0	142
3	A Modern First-Principles View on Ligand Field Theory Through the Eyes of Correlated Multireference Wavefunctions. Structure and Bonding, 2011, , 149-220.	1.0	94
4	Theoretical Determination of the Zero-Field Splitting in Copper Acetate Monohydrate. Inorganic Chemistry, 2011, 50, 6229-6236.	4.0	91
5	Systematic Theoretical Study of the Zero-Field Splitting in Coordination Complexes of Mn(III). Density Functional Theory versus Multireference Wave Function Approaches. Journal of Physical Chemistry A, 2010, 114, 10750-10758.	2.5	129
6	The resolution of the identity approximation for calculations of spin-spin contribution to zero-field splitting parameters. Journal of Chemical Physics, 2010, 132, 144111.	3.0	49
7	A Multiconfigurational ab Initio Study of the Zero-Field Splitting in the Di- and Trivalent Hexaquoâ^'Chromium Complexes. Inorganic Chemistry, 2009, 48, 10572-10580.	4.0	54
8	Direct Detection and Characterization of Chloride in the Active Site of the Low-pH Form of Sulfite Oxidase Using Electron Spin Echo Envelope Modulation Spectroscopy, Isotopic Labeling, and Density Functional Theory Calculations. Inorganic Chemistry, 2009, 48, 4743-4752.	4.0	33
9	Multireference ab initio studies of zero-field splitting and magnetic circular dichroism spectra of tetrahedral Co(ii) complexes. Dalton Transactions, 2009, , 6021.	3.3	64
10	Exchangeable oxygens in the vicinity of the molybdenum center of the high-pH form of sulfite oxidase and sulfite dehydrogenase. Physical Chemistry Chemical Physics, 2009, 11, 6733.	2.8	22
11	First-principles calculations of magnetic circular dichroism spectra. Journal of Chemical Physics, 2008, 128, 114117.	3.0	86
12	Advanced aspects of ab initio theoretical optical spectroscopy of transition metal complexes: Multiplets, spin-orbit coupling and resonance Raman intensities. Coordination Chemistry Reviews, 2007, 251, 288-327.	18.8	285
13	First-principles calculations of zero-field splitting parameters. Journal of Chemical Physics, 2006, 125, 024103.	3.0	322