Steven Vancoillie

List of Publications by Year
in descending order

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22 papers	3,286 citations	471509 17 h-index	713466 21 g-index
22 all docs	22 docs citations	22 times ranked	3757 citing authors

#	Article	IF	Citations
1	<scp>Molcas</scp> 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. Journal of Computational Chemistry, 2016, 37, 506-541.	3.3	1,317
2	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	5.3	661
3	Relative energy of the high-(T2g5) and low-(A1g1) spin states of [Fe(H2O)6]2+, [Fe(NH3)6]2+, and [Fe(bpy)3]2+: CASPT2 versus density functional theory. Journal of Chemical Physics, 2006, 125, 124303.	3.0	178
4	Multiconfigurational Second-Order Perturbation Theory Restricted Active Space (RASPT2) Method for Electronic Excited States: A Benchmark Study. Journal of Chemical Theory and Computation, 2011, 7, 153-168.	5.3	164
5	Performance of CASPT2 and DFT for Relative Spin-State Energetics of Heme Models. Journal of Chemical Theory and Computation, 2010, 6, 576-582.	5.3	147
6	Relative energy of the high-(T2g5) and low-(A1g1) spin states of the ferrous complexes [Fe(L)(NHS4)]: CASPT2 versus density functional theory. Journal of Chemical Physics, 2008, 128, 034104.	3.0	132
7	Multiconfigurational Second-Order Perturbation Theory Restricted Active Space (RASPT2) Studies on Mononuclear First-Row Transition-Metal Systems. Journal of Chemical Theory and Computation, 2011, 7, 3961-3977.	5.3	118
8	Calculation of EPR g Tensors for Transitionâ€Metal Complexes Based on Multiconfigurational Perturbation Theory (CASPT2). ChemPhysChem, 2007, 8, 1803-1815.	2.1	85
9	Copper Corroles: the Question of Noninnocence. Inorganic Chemistry, 2010, 49, 10316-10329.	4.0	83
10	Theoretical Description of the Structure and Magnetic Properties of Nitroxideâ^'Cu(II)â^'Nitroxide Spin Triads by Means of Multiconfigurational Ab Initio Calculations. Journal of Physical Chemistry A, 2009, 113, 6149-6157.	2.5	60
11	Accurate calculations of geometries and singletâ€“triplet energy differences for active-site models of [NiFe] hydrogenase. Physical Chemistry Chemical Physics, 2014, 16, 7927-7938.	2.8	58
12	Multiconfigurational g Tensor Calculations as a Probe for the Covalency of the Copperâ^'Ligand Bonds in Copper(II) Complexes:â€‰ [CuCl₄]²⁻, [Cu(NH₃)₄]²⁺, and Plastocyanin. Journal of Physical Chemistry A, 2008, 112, 4011-4019.	2.5	52
13	Potential Energy Surface of the Chromium Dimer Re-re-revisited with Multiconfigurational Perturbation Theory. Journal of Chemical Theory and Computation, 2016, 12, 1647-1655.	5.3	49
14	A Multiconfigurational Perturbation Theory and Density Functional Theory Study on the Heterolytic Dissociation Enthalpy of First-Row Metallocenes. Journal of Chemical Theory and Computation, 2012, 8, 883-892.	5.3	45
15	Multireference Ab Initio Calculations of g tensors for Trinuclear Copper Clusters in Multicopper Oxidases. Journal of Physical Chemistry B, 2010, 114, 7692-7702.	2.6	42
16	Parallelization of a multiconfigurational perturbation theory. Journal of Computational Chemistry, 2013, 34, 1937-1948.	3.3	35
17	Electronic Spectra ofN-Heterocyclic Pentacyanoferrate(II) Complexes in Different Solvents, Studied by Multiconfigurational Perturbation Theory. Inorganic Chemistry, 2013, 52, 10653-10663.	4.0	22
18	Theoretical Study of the Dissociation Energy of First-Row Metallocenium Ions. Journal of Chemical Theory and Computation, 2014, 10, 3681-3688.	5.3	15

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19	Fourteen-Electron Ring Model and the Anomalous Magnetic Circular Dichroism of meso-Triarylsubporphyrins. Journal of Physical Chemistry A, 2012, 116, 3960-3967.	2.5	10
20	Ruthenocene and cyclopentadienyl pyrrolyl ruthenium as precursors for ruthenium atomic layer deposition: a comparative study of dissociation enthalpies. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	8
21	A multiconfigurational perturbation theory study of the electronic structure and EPR g values of an oxomolybdenum enzyme model complex. Theoretical Chemistry Accounts, 2009, 124, 251-259.	1.4	5
22	Ruthenocene and cyclopentadienyl pyrrolyl ruthenium as precursors for ruthenium atomic layer deposition: a comparative study of dissociation enthalpies. Highlights in Theoretical Chemistry, 2014, , 61-69.	0.0	0