

Steven Vancoillie

List of Publications by Year in descending order

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22
papers

3,286
citations

471509

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713466

21
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all docs

22
docs citations

22
times ranked

3757
citing authors

#	ARTICLE	IF	CITATIONS
1	OpenMolcas: From Source Code to Insight. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5925-5964.	5.3	661
2	<scp>Molcas</scp> 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. <i>Journal of Computational Chemistry</i> , 2016, 37, 506-541.	3.3	1,317
3	Potential Energy Surface of the Chromium Dimer Re-re-visited with Multiconfigurational Perturbation Theory. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1647-1655.	5.3	49
4	Theoretical Study of the Dissociation Energy of First-Row Metallocenium Ions. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3681-3688.	5.3	15
5	Accurate calculations of geometries and singlet-triplet energy differences for active-site models of [NiFe] hydrogenase. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 7927-7938.	2.8	58
6	Ruthenocene and cyclopentadienyl pyrrolyl ruthenium as precursors for ruthenium atomic layer deposition: a comparative study of dissociation enthalpies. <i>Highlights in Theoretical Chemistry</i> , 2014, , 61-69.	0.0	0
7	Electronic Spectra of N-Heterocyclic Pentacyanoferrate(II) Complexes in Different Solvents, Studied by Multiconfigurational Perturbation Theory. <i>Inorganic Chemistry</i> , 2013, 52, 10653-10663.	4.0	22
8	Parallelization of a multiconfigurational perturbation theory. <i>Journal of Computational Chemistry</i> , 2013, 34, 1937-1948.	3.3	35
9	Fourteen-Electron Ring Model and the Anomalous Magnetic Circular Dichroism of <i>meso</i> -Triarylsubporphyrins. <i>Journal of Physical Chemistry A</i> , 2012, 116, 3960-3967.	2.5	10
10	A Multiconfigurational Perturbation Theory and Density Functional Theory Study on the Heterolytic Dissociation Enthalpy of First-Row Metallocenes. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 883-892.	5.3	45
11	Ruthenocene and cyclopentadienyl pyrrolyl ruthenium as precursors for ruthenium atomic layer deposition: a comparative study of dissociation enthalpies. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	1.4	8
12	Multiconfigurational Second-Order Perturbation Theory Restricted Active Space (RASPT2) Method for Electronic Excited States: A Benchmark Study. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 153-168.	5.3	164
13	Multiconfigurational Second-Order Perturbation Theory Restricted Active Space (RASPT2) Studies on Mononuclear First-Row Transition-Metal Systems. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3961-3977.	5.3	118
14	Copper Corroles: the Question of Noninnocence. <i>Inorganic Chemistry</i> , 2010, 49, 10316-10329.	4.0	83
15	Multireference Ab Initio Calculations of $\langle b \rangle g \langle b \rangle$ tensors for Trinuclear Copper Clusters in Multicopper Oxidases. <i>Journal of Physical Chemistry B</i> , 2010, 114, 7692-7702.	2.6	42
16	Performance of CASPT2 and DFT for Relative Spin-State Energetics of Heme Models. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 576-582.	5.3	147
17	A multiconfigurational perturbation theory study of the electronic structure and EPR g values of an oxomolybdenum enzyme model complex. <i>Theoretical Chemistry Accounts</i> , 2009, 124, 251-259.	1.4	5
18	Theoretical Description of the Structure and Magnetic Properties of Nitroxide-Cu(II)-Nitroxide Spin Triads by Means of Multiconfigurational Ab Initio Calculations. <i>Journal of Physical Chemistry A</i> , 2009, 113, 6149-6157.	2.5	60

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19	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
20	Multiconfigurational g Tensor Calculations as a Probe for the Covalency of the Copper ^{II} Ligand Bonds in Copper(II) Complexes: [CuCl ₄] ²⁻ , [Cu(NH ₃) ₃] ²⁺ , and Plastocyanin. Journal of Physical Chemistry A, 2008, 112, 4011-4019.	2.5	52
21	Calculation of EPR g Tensors for Transition-Metal Complexes Based on Multiconfigurational Perturbation Theory (CASPT2). ChemPhysChem, 2007, 8, 1803-1815.	2.1	85
22	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