

Second-order perturbation theory with a CASSCF reference

The Journal of Physical Chemistry

94, 5483-5488

DOI: 10.1021/j100377a012

Citation Report

#	ARTICLE	IF	CITATIONS
23	First-order correlation orbitals for the MCSCF zeroth-order wave function. <i>Chemical Physics Letters</i> , 1991, 183, 483-490.	1.2	1
24	A theoretical study of the CuOH molecule. <i>Chemical Physics Letters</i> , 1991, 185, 535-543.	1.2	12
25	Generalized Møller-Plesset perturbation theory applied to general MCSCF reference wave functions. <i>Chemical Physics Letters</i> , 1991, 183, 443-448.	1.2	145
26	Error analysis and improvements of coupled-cluster theory. <i>Theoretica Chimica Acta</i> , 1991, 80, 349-386.	0.9	142
27	Correlated studies of electric properties of ionic molecules: alkali and alkaline-earth hydrides, halides and chalcogenides. <i>Molecular Physics</i> , 1991, 73, 43-55.	0.8	47
28	Vibrational frequencies of ozone: A multiconfigurational approach. <i>Journal of Chemical Physics</i> , 1992, 97, 5568-5577.	1.2	77
29	Comparison and assessment of different forms of open shell perturbation theory. <i>Journal of Chemical Physics</i> , 1992, 97, 6509-6516.	1.2	51
30	Electric dipole polarizabilities of atomic valence states. <i>Physical Review A</i> , 1992, 46, 2356-2362.	1.0	68
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32	Chapter 3. Theoretical organic chemistry. <i>Annual Reports on the Progress of Chemistry Section B</i> , 1992, 89, 35.	0.8	1
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38	Excitation energies in the nickel atom studied with the complete active space SCF method and second-order perturbation theory. <i>Chemical Physics Letters</i> , 1992, 191, 507-514.	1.2	198
39	Ab initio quantum-chemical study of the lower-lying electronic states of o-benzyne. <i>Chemical Physics Letters</i> , 1992, 198, 259-265.	1.2	16
40	Multireference Møller-Plesset method. <i>Chemical Physics Letters</i> , 1992, 190, 374-380.	1.2	661

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42	Long bonds in silicon clusters: a failure of conventional MÅller-Plesset perturbation theory?. <i>Chemical Physics Letters</i> , 1992, 192, 277-282.	1.2	22
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1954	QM/MM studies on the excited-state relaxation mechanism of a semisynthetic dTPT3 base. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 5067-5073.	1.3	11
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1957	Crystal Field in Rare-Earth Complexes: From Electrostatics to Bonding. <i>Chemistry - A European Journal</i> , 2018, 24, 5538-5550.	1.7	21
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1959	Analytic Gradients for Complete Active Space Pair-Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 126-138.	2.3	40
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1974	Understanding the Mechanism Stabilizing Intermediate Spin States in Fe(II)-Porphyrin. <i>Journal of Physical Chemistry A</i> , 2018, 122, 4935-4947.	1.1	75
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1980	Mechanistic Insights into Photocatalyzed Hydrogen Desorption from Palladium Surfaces Assisted by Localized Surface Plasmon Resonances. <i>ACS Nano</i> , 2018, 12, 3512-3522.	7.3	62
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1982	Development of Xi'an-CI package applying the hole-particle symmetry in multi-reference electronic correlation calculations. <i>Molecular Physics</i> , 2018, 116, 1051-1064.	0.8	18
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1985	Evolutionary algorithm based configuration interaction approach. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25509.	1.0	11
1986	Excited-state proton transfer induced [4 + 2] and [4 + 4] photocycloaddition reactions of an oxazoline: Mechanism and selectivity. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2018, 355, 256-266.	2.0	4
1987	Mechanistic insights into photoinduced damage of DNA and RNA nucleobases in the gas phase and in bulk solution. <i>Faraday Discussions</i> , 2018, 207, 329-350.	1.6	10
1988	Exchange Coupling Interactions from the Density Matrix Renormalization Group and <i>i</i> -N-Electron Valence Perturbation Theory: Application to a Biomimetic Mixed-Valence Manganese Complex. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 166-179.	2.3	62
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1993	Direct diabaticization based on nonadiabatic couplings: the N/D method. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 26643-26659.	1.3	12
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1995	Mechanisms of Bisphosphine Iron-Catalyzed C(SP ²)-C(SP ³) Cross-Coupling Reactions: Inner-Sphere or Outer-Sphere Arylation?. <i>Comments on Inorganic Chemistry</i> , 2018, 38, 210-237.	3.0	8
1996	Exact and approximate adiabatic connection formulae for the correlation energy in multireference ground and excited states. <i>Journal of Chemical Physics</i> , 2018, 149, 204101.	1.2	20
1997	Electronic Excitations in Complex Molecular Environments: Many-Body Green's Functions Theory in VOTCA-XTP. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 6253-6268.	2.3	28
1998	A linear cobalt(II) complex with maximal orbital angular momentum from a non-Aufbau ground state. <i>Science</i> , 2018, 362, .	6.0	254
1999	Preferential Photoreaction in a Porous Crystal, Metal- <i>ſ</i> Macrocycle Framework: Pd ^{II} -Mediated Olefin Migration over [2+2] Cycloaddition. <i>Journal of the American Chemical Society</i> , 2018, 140, 16610-16614.	6.6	29
2000	Open-shell coupled-cluster valence-bond theory augmented with an independent amplitude approximation for three-pair correlations: Application to a model oxygen-evolving complex and single molecular magnet. <i>Journal of Chemical Physics</i> , 2018, 149, 244121.	1.2	13
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2016	Fermi-Landau orbital self-interaction correction to magnetic exchange couplings. <i>Journal of Chemical Physics</i> , 2018, 149, 164101.	1.2	33
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2028	Coordination of N ₂ ligands to lanthanum: the complexes La (N ₂) ₁₋₈ . <i>Structural Chemistry</i> , 2018, 29, 1825-1837.	1.0	6
2029	Excited-State Decay Pathways of Flavin Molecules in Five Redox Forms: The Role of Conical Intersections. <i>Journal of Physical Chemistry A</i> , 2018, 122, 7954-7961.	1.1	15
2030	Post Hartree-Fock calculations of pnictogen-uranium bonding in EUF ₃ (E = N, Bi). <i>Chemical Communications</i> , 2018, 54, 11100-11103.	2.2	6
2031	Development of approximate spin projection method and its application for elucidation of electronic structures, molecular structures and physical properties of polynuclear metal complexes. <i>Bulletin of Japan Society of Coordination Chemistry</i> , 2018, 71, 57-68.	0.1	0
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2035	Origin of the green persistent luminescence of Eu-doped SrAl ₂ O ₄ from a multiconfigurational <i>ab initio</i> study of 4f ^{sup>7</sup>â†’4f^{sup>6</sup>5d^{sup>1</sup> transitions. <i>Journal of Materials Chemistry C</i>, 2018, 6, 6637-6640.}}}	2.7	40
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2037	Zero-point energy conservation in classical trajectory simulations: Application to H ₂ CO. <i>Journal of Chemical Physics</i> , 2018, 148, 194113.	1.2	13

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2039	OMS, OM(\hat{i} -2-SO), and OM(\hat{i} -2-SO)(\hat{i} -2-O2S) Molecules (M = Ce, Th) with Chiral Structure: Matrix Infrared Spectra and Theoretical Calculations. <i>Journal of Physical Chemistry A</i> , 2018, 122, 5391-5400.	1.1	3
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2042	Linear-Response Density Cumulant Theory for Excited Electronic States. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4097-4108.	2.3	8
2043	A Mountaineering Strategy to Excited States: Highly Accurate Reference Energies and Benchmarks. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4360-4379.	2.3	211
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2051	The effect of substituents on energy splitting in organic radicals: Quantitative cognizance from ab initio studies. <i>Chemical Physics</i> , 2018, 513, 230-240.	0.9	0
2052	Reduced scaling CASPT2 using supporting subspaces and tensor hyper-contraction. <i>Journal of Chemical Physics</i> , 2018, 149, 044108.	1.2	31
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2054	Pentavalent Curium, Berkelium, and Californium in Nitrate Complexes: Extending Actinide Chemistry and Oxidation States. <i>Inorganic Chemistry</i> , 2018, 57, 9453-9467.	1.9	15
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2057	Combining Wave Function Methods with Density Functional Theory for Excited States. <i>Chemical Reviews</i> , 2018, 118, 7249-7292.	23.0	166
2058	Mechanistical Insights into the Bioconjugation Reaction of Triazolinediones with Tyrosine. <i>Journal of Organic Chemistry</i> , 2018, 83, 10248-10260.	1.7	15
2059	State-interaction pair-density functional theory. <i>Journal of Chemical Physics</i> , 2018, 149, 024106.	1.2	27
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2061	Computational modelling of singlet excitation energy transfer: a DFT/TD-DFT study of the ground and excited state properties of a syn bimeane dimer system using non-empirically tuned range-separated functionals. <i>New Journal of Chemistry</i> , 2018, 42, 13732-13743.	1.4	2
2062	Perspective: Multireference coupled cluster theories of dynamical electron correlation. <i>Journal of Chemical Physics</i> , 2018, 149, 030901.	1.2	96
2063	A quantitative tool to establish magic number clusters, $\hat{\mu}_3$, applied in small silicon clusters, Si ₂ -11. <i>Journal of Molecular Modeling</i> , 2018, 24, 203.	0.8	7
2064	Automatic Differentiation in Quantum Chemistry with Applications to Fully Variational Hartree-Fock. <i>ACS Central Science</i> , 2018, 4, 559-566.	5.3	57
2065	Excited state dynamics and time-resolved photoelectron spectroscopy of <i>p</i> -xylylene. <i>Faraday Discussions</i> , 2018, 212, 83-100.	1.6	6
2066	Nonadiabatic dynamics: The SHARC approach. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2018, 8, e1370.	6.2	274
2067	Thermodynamic Stabilities, Electronic Properties, and Optical Transitions of Intrinsic Defects and Lanthanide Ions (Ce ³⁺ , Eu ²⁺ , and Eu ³⁺) in Li ₂ SrSiO ₄ . <i>Inorganic Chemistry</i> , 2018, 57, 6142-6151.	1.9	20
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2069	Kinetics of reaction $RH + O_2 = R + HO_2$ ($RH = \text{normal C}_{14}$ alkanes): A DFT investigation. <i>Fuel</i> , 2018, 234, 1165-1172.	3.4	6
2070	Comparative study of the photodynamics of malonaldehyde and acetylacetone. <i>Chemical Physics</i> , 2018, 515, 622-627.	0.9	3
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