Celestino Angeli

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/7826570/publications.pdf

Version: 2024-02-01

116 papers	8,551 citations	126901 33 h-index	43886 91 g-index
119 all docs	119 docs citations	119 times ranked	5574 citing authors

#	Article	IF	Citations
1	Introduction ofn-electron valence states for multireference perturbation theory. Journal of Chemical Physics, 2001, 114, 10252-10264.	3.0	1,386
2	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	14.6	1,166
3	n-electron valence state perturbation theory: A spinless formulation and an efficient implementation of the strongly contracted and of the partially contracted variants. Journal of Chemical Physics, 2002, 117, 9138-9153.	3.0	911
4	N-electron valence state perturbation theory: a fast implementation of the strongly contracted variant. Chemical Physics Letters, 2001, 350, 297-305.	2.6	689
5	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	5.3	661
6	A quasidegenerate formulation of the second order n-electron valence state perturbation theory approach. Journal of Chemical Physics, 2004, 121, 4043-4049.	3.0	313
7	New perspectives in multireference perturbation theory: the n-electron valence state approach. Theoretical Chemistry Accounts, 2007, 117, 743-754.	1.4	238
8	Shape of Multireference, Equation-of-Motion Coupled-Cluster, and Density Functional Theory Potential Energy Surfaces at a Conical Intersection. Journal of Chemical Theory and Computation, 2014, 10, 3074-3084.	5.3	161
9	Third-order multireference perturbation theory: The n-electron valence state perturbation-theory approach. Journal of Chemical Physics, 2006, 124, 054108.	3.0	151
10	Dynamic Electron Correlation Effects on the Ground State Potential Energy Surface of a Retinal Chromophore Model. Journal of Chemical Theory and Computation, 2012, 8, 4069-4080.	5.3	149
11	Analysis of the magnetic coupling in binuclear systems. III. The role of the ligand to metal charge transfer excitations revisited. Journal of Chemical Physics, 2009, 131, 044327.	3.0	110
12	On the nature of the Ï€ â†' Ï€* ionic excited states: The V state of ethene as a prototype. Journal of Computational Chemistry, 2009, 30, 1319-1333.	3.3	109
13	Multireference Perturbation Theory with Cholesky Decomposition for the Density Matrix Renormalization Group. Journal of Chemical Theory and Computation, 2017, 13, 451-459.	5.3	88
14	On the applicability of multireference secondâ€•order perturbation theory to study weak magnetic coupling in molecular complexes. Journal of Computational Chemistry, 2008, 29, 994-1003.	3.3	84
15	Mapping the Excited State Potential Energy Surface of a Retinal Chromophore Model with Multireference and Equation-of-Motion Coupled-Cluster Methods. Journal of Chemical Theory and Computation, 2013, 9, 4495-4506.	5.3	83
16	Multireference perturbation configuration interaction V. Third-order energy contributions in the Mï¿½ller?Plesset and Epstein?Nesbet partitions. Theoretical Chemistry Accounts, 2002, 107, 313-317.	1.4	69
17	Bond electron pair: Its relevance and analysis from the quantum chemistry point of view. Journal of Computational Chemistry, 2007, 28, 35-50.	3.3	64
18	A novel perturbation-based complete active spaceâ€“self-consistent-field algorithm: Application to the direct calculation of localized orbitals. Journal of Chemical Physics, 2002, 117, 10525-10533.	3.0	61

#	Article	IF	Citations
19	Multireference perturbation CI I. Extrapolation procedures with CAS or selected zero-order spaces. Theoretical Chemistry Accounts, 1997, 98, 57-63.	1.4	57
20	Metalâ€“Metal Interactions in Trinuclear Copper(II) Complexes [Cu₃(RCOO)₄(H₂TEA)₂] and Binuclear [Cu₂(RCOO)₂(H₂TEA)₂]. Syntheses and Combined Structural, Magnetic, High-Field Electron Paramagnetic Resonance, and Theoretical Studies. Inorganic Chemistry, 2015, 54, 11916-11934.	4.0	56
21	Multireference perturbation CI II. Selection of the zero-order space. Theoretical Chemistry Accounts, 1997, 98, 117-128.	1.4	54
22	A one-dimensional numerical study of the salt diffusion in a salinity-gradient solar pond. International Journal of Heat and Mass Transfer, 2004, 47, 1-10.	4.8	51
23	The lowest singlet states of octatetraene revisited. Journal of Chemical Physics, 2011, 134, 184302.	3.0	51
24	Calibration of the n-electron valence state perturbation theory approach. Journal of Chemical Physics, 2004, 120, 4619-4625.	3.0	49
25	Excitation energies of retinal chromophores: critical role of the structural model. Physical Chemistry Chemical Physics, 2012, 14, 11015.	2.8	48
26	On the Relative Merits of Non-Orthogonal and Orthogonal Valence Bond Methods Illustrated on the Hydrogen Molecule. Journal of Chemical Education, 2008, 85, 150.	2.3	47
27	Beryllium Dimer: A Bond Based on Non-Dynamical Correlation. Journal of Physical Chemistry A, 2014, 118, 6664-6673.	2.5	44
28	On a mixed MÃ¸llerâ€“Plesset Epsteinâ€“Nesbet partition of the Hamiltonian to be used in multireference perturbation configuration interaction. Chemical Physics Letters, 2000, 317, 472-480.	2.6	41
29	A convenient decontraction procedure of internally contracted state-specific multireference algorithms. Journal of Chemical Physics, 2006, 124, 234109.	3.0	41
30	The role of the magnetic orbitals in the calculation of the magnetic coupling constants from multireference perturbation theory methods. Journal of Chemical Physics, 2012, 137, 034104.	3.0	41
31	Density Relaxation in Time-Dependent Density Functional Theory: Combining Relaxed Density Natural Orbitals and Multireference Perturbation Theories for an Improved Description of Excited States. Journal of Chemical Theory and Computation, 2014, 10, 4014-4024.	5.3	41
32	The use of local orbitals in multireference calculations. Molecular Physics, 2003, 101, 1389-1398.	1.7	36
33	An application of second-order n-electron valence state perturbation theory to the calculation of excited states. Theoretical Chemistry Accounts, 2004, 111, 352-357.	1.4	35
34	The effect of thermodiffusion on the stability of a salinity gradient solar pond. International Journal of Heat and Mass Transfer, 2005, 48, 4633-4639.	4.8	33
35	The vertical electronic spectrum of pyrrole: A second and third order n-electron valence state perturbation theory study. Chemical Physics Letters, 2006, 422, 522-528.	2.6	32
36	Dynamical photoionization observables of the CS molecule: The role of electron correlation. Journal of Chemical Physics, 2014, 140, 204304.	3.0	32

#	Article	IF	Citations
37	Ground states of the Mo2, W2, and CrMo molecules: A second and third order multireference perturbation theory study. Journal of Chemical Physics, 2007, 127, 074306.	3.0	31
38	The problem of interoperability: A common data format for quantum chemistry codes. International Journal of Quantum Chemistry, 2007, 107, 2082-2091.	2.0	31
39	Analysis of the magnetic coupling in nitroxide organic biradicals. Theoretical Chemistry Accounts, 2011, 128, 505-519.	1.4	31
40	Metal-to-metal charge-transfer transitions: reliable excitation energies from ab initio calculations. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	31
41	Ab initio n-electron valence state perturbation theory study of the adiabatic transitions in carbonyl molecules: Formaldehyde, acetaldehyde, and acetone. Journal of Chemical Physics, 2005, 122, 114304.	3.0	30
42	A computational study of salt diffusion and heat extraction in solar pond plants. Solar Energy, 2006, 80, 1498-1508.	6.1	30
43	FORTRAN Interface for Code Interoperability in Quantum Chemistry:â€‰ The Q5Cost Library. Journal of Chemical Information and Modeling, 2007, 47, 1271-1277.	5.4	29
44	On the competition between the inversion and rotation mechanisms in the cis-trans thermal isomerization of diazene. Chemical Physics Letters, 1996, 259, 276-282.	2.6	28
45	X-ray absorption and resonant Auger spectroscopy of O2 in the vicinity of the O 1sâ†'Ïƒ* resonance: Experiment and theory. Journal of Chemical Physics, 2008, 128, 064304.	3.0	28
46	A perturbationâ€based superâ€CI approach for the orbital optimization of a CASSCF wave function. Journal of Computational Chemistry, 2019, 40, 1463-1470.	3.3	28
47	An ab initio multireference perturbation theory study on the manganese dimer. Journal of Chemical Physics, 2008, 128, 244317.	3.0	27
48	On the controversial nature of the 1â€‰B1u and 2â€‰B1u states of trans-stilbene: The n-electron valence state perturbation theory approach. Journal of Chemical Physics, 2009, 130, 174307.	3.0	27
49	Charge-displacement analysis for excited states. Journal of Chemical Physics, 2014, 140, 054110.	3.0	26
50	Magnetic behaviour vs. structural changes in an isomeric series of binuclear copper(<scp>ii</scp>) complexes: an experimental and theoretical study. New Journal of Chemistry, 2014, 38, 574-583.	2.8	26
51	Electronic structure investigation of the evanescent AtO⁺ion. Physical Chemistry Chemical Physics, 2014, 16, 9238-9248.	2.8	25
52	A Jeziorski-Monkhorst fully uncontracted multi-reference perturbative treatment. I. Principles, second-order versions, and tests on ground state potential energy curves. Journal of Chemical Physics, 2017, 146, 224108.	3.0	25
53	Threshold Photoionization Study of Fe(CO)5versus ab Initio Calculations. Journal of Physical Chemistry A, 1997, 101, 7907-7913.	2.5	24
54	Can the second order multireference perturbation theory be considered a reliable tool to study mixed-valence compounds?. Journal of Chemical Physics, 2008, 128, 174102.	3.0	24

#	Article	IF	Citations
55	Extending the active space in multireference configuration interaction calculations of magnetic coupling constants. Theoretical Chemistry Accounts, 2010, 126, 185-196.	1.4	24
56	On the Maxwellâ˜Stefan Approach to Diffusion: A General Resolution in the Transient Regime for One-Dimensional Systems. Journal of Physical Chemistry B, 2010, 114, 151-164.	2.6	24
57	The electronic structure of Ullman's biradicals: an orthogonal valence bond interpretation. Physical Chemistry Chemical Physics, 2011, 13, 14617.	2.8	24
58	Quasi-bond orbitals from maximum-localization hybrids for ab initio CI calculations. Chemical Physics Letters, 1995, 233, 102-110.	2.6	23
59	A multireference perturbation theory study on the vertical electronic spectrum of thiophene. Theoretical Chemistry Accounts, 2007, 118, 35-46.	1.4	23
60	A multireference perturbation theory study on the Fe₂molecule: in quest of the ground state. Molecular Physics, 2011, 109, 1503-1509.	1.7	23
61	Multiple complete active space self-consistent field solutions. Molecular Physics, 2003, 101, 1937-1944.	1.7	22
62	A comparison of various approaches in internally contracted multireference configuration interaction: the carbon dimer as a test case. Molecular Physics, 2012, 110, 2963-2968.	1.7	22
63	Code interoperability and standard data formats in quantum chemistry and quantum dynamics: The Q5/D5Cost data model. Journal of Computational Chemistry, 2014, 35, 611-621.	3.3	22
64	Constant-atomic-final-state filtering of dissociative states in the O1sâ†'Ïƒ* core excitation in O2. Journal of Chemical Physics, 2005, 123, 064314.	3.0	20
65	An application of second and third-order n-electron valence state perturbation theory to the calculation of the vertical electronic spectrum of furan. Chemical Physics Letters, 2006, 426, 445-451.	2.6	20
66	Improving the calculation of magnetic coupling constants in MRPT methods. Journal of Computational Chemistry, 2014, 35, 1665-1671.	3.3	20
67	Photoionization of furan from the ground and excited electronic states. Journal of Chemical Physics, 2016, 144, 084307.	3.0	20
68	O1sâ†'Ïƒ*Resonance inO2: Inadequacy of Only Two Exchange-Split Components. Physical Review Letters, 2002, 88, 243002.	7.8	19
69	Non-orthogonal and orthogonal valence bond wavefunctions in the hydrogen molecule: the diabatic view. Molecular Physics, 2013, 111, 1069-1077.	1.7	19
70	Behavior of the Positionâ€“Spread Tensor in Diatomic Systems. Journal of Chemical Theory and Computation, 2013, 9, 5286-5295.	5.3	19
71	Multireference perturbation CI III. Fast evaluation of the one-particle density matrix. Theoretical Chemistry Accounts, 1998, 100, 324-328.	1.4	18
72	A CASSCF theoretical study of the vibrational frequencies and structure of formaldehyde, acetaldehyde and acetone valence excited states. Computational and Theoretical Chemistry, 2005, 718, 55-69.	1.5	18

#	Article	IF	Citations
73	Metal-ligand delocalization and spin density in the CuCl2 and [CuCl4]2â^' molecules: Some insights from wave function theory. Journal of Chemical Physics, 2015, 143, 124305.	3.0	18
74	Aromaticity: an ab Initio Evaluation of the Properly Cyclic Delocalization Energy and the Ï€-Delocalization Energy Distortivity of Benzene. Journal of Physical Chemistry A, 2008, 112, 11481-11486.	2.5	17
75	Quasi-diabatic and adiabatic states and potential energy curves for Naî—¸Cd collisions and excimer formation. Chemical Physics, 1996, 204, 57-64.	1.9	16
76	An analysis of the dynamic Ïƒ polarization in the V state of ethene. International Journal of Quantum Chemistry, 2010, 110, 2436-2447.	2.0	16
77	Highly efficient perturbative + variational strategy based on orthogonal valence bond theory for the evaluation of magnetic coupling constants. Application to the trinuclear Cu(<scp>II</scp>) site of multicopper oxidases. Physical Chemistry Chemical Physics, 2016, 18, 18365-18380.	2.8	16
78	Multireference perturbation CI IV. Selection procedure for one-electron properties. Theoretical Chemistry Accounts, 2001, 105, 259-264.	1.4	15
79	The Effect of the Basis-Set Superposition Error on the Calculation of Dispersion Interactions:â€‰ A Test Study on the Neon Dimer. Journal of Chemical Theory and Computation, 2007, 3, 477-485.	5.3	15
80	A Simple Approximate Perturbation Approach to Quasi-degenerate Systems. Theoretical Chemistry Accounts, 2006, 116, 434-439.	1.4	14
81	â€œCagingâ€•Anions through Crystal Engineering to Avoid Polymerization: Structural, Conformational and Theoretical Investigations of New Halocadmate [Cd2X7]3- Anions (X = Cl/Br). European Journal of Inorganic Chemistry, 2012, 2012, 1195-1203.	2.0	14
82	Electronic reorganization triggered by electron transfer: The intervalence charge transfer of a Fe³⁺/Fe²⁺ bimetallic complex. Journal of Computational Chemistry, 2015, 36, 861-869.	3.3	14
83	Developments in then-electron valence state perturbation theory. International Journal of Quantum Chemistry, 2006, 106, 686-691.	2.0	13
84	A theoretical study of BeN linear chains: Variational and perturbative approaches. Journal of Chemical Physics, 2009, 131, 034309.	3.0	13
85	The localization tensor for the H2 molecule: Closed formulae for the Heitler-London and related wavefunctions and comparison with full configuration interaction. Journal of Chemical Physics, 2013, 138, 054314.	3.0	13
86	Assessment of Multireference Perturbation Methods for Chemical Reaction Barrier Heights. Journal of Physical Chemistry A, 2015, 119, 5490-5495.	2.5	13
87	A multireference n-electron Valence State Perturbation Theory study of the electronic spectrum of s-tetrazine. Theoretical Chemistry Accounts, 2009, 123, 287-298.	1.4	12
88	Optical absorption spectrum of the N3 solar cell sensitizer by second-order multireference perturbation theory. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	11
89	Common Format for Quantum Chemistry Interoperability: Q5Cost Format and Library. Lecture Notes in Computer Science, 2008, , 1094-1107.	1.3	11
90	Application of a â€œcharge-averagedâ€•second order multireference perturbation theory strategy to the study of a model Mixed-Valence compound. Computational and Theoretical Chemistry, 2009, 896, 12-17.	1.5	10

#	Article	IF	Citations
91	Physical Interpretation of Koopmans' Theorem: A Criticism of the Current Didactic Presentation. Journal of Chemical Education, 1998, 75, 1494.	2.3	9
92	Geometry optimization within a localized CAS-SCF approach. Chemical Physics Letters, 2003, 371, 49-55.	2.6	9
93	Spin density and orbital optimization in open shell systems: A rational and computationally efficient proposal. Journal of Chemical Physics, 2016, 144, 104104.	3.0	9
94	Strongly localized approaches for delocalized systems. I. Ground state of linear polyenes. Computational and Theoretical Chemistry, 2017, 1116, 102-111.	2.5	9
95	Local orbitals for quasi-degenerate systems. Computational and Theoretical Chemistry, 2004, 709, 1-10.	1.5	8
96	The Intriguing Case of the Oneâ€Photon and Twoâ€Photon Absorption of a Prototypical Symmetric Squaraine: Comparison of TDDFT and Waveâ€Function Methods. ChemPhotoChem, 2019, 3, 778-793.	3.0	8
97	Computer assisted generation of the matrix elements between contracted wavefunctions in a Complete Active Space scheme. Computer Physics Communications, 2005, 166, 53-57.	7.5	7
98	Influence of the interaction potential and of the temperature on the thermodiffusion (Soret) coefficient in a model system. Journal of Chemical Physics, 2008, 128, 054507.	3.0	7
99	The Spin-Partitioned Total-Position Spread Tensor: An Application To Diatomic Molecules. Journal of Physical Chemistry A, 2016, 120, 5230-5238.	2.5	7
100	Transient Diffusion within Spherical Particles: Numerical Resolution of the Maxwellâ^'Stefan Formulation. Industrial & Engineering Chemistry Research, 2010, 49, 5654-5660.	3.7	6
101	The MÃ¸llerâ€“Plesset perturbation revisited: origin of high-order divergences. Molecular Physics, 2013, 111, 1092-1099.	1.7	6
102	The â€œFermi holeâ€•and the correlation introduced by the symmetrization or the anti-symmetrization of the wave function. Journal of Chemical Physics, 2016, 145, 124114.	3.0	6
103	Computation of the Isotropic Hyperfine Coupling Constant: Efficiency and Insights from a New Approach Based on Wave Function Theory. Journal of Chemical Theory and Computation, 2017, 13, 475-487.	5.3	6
104	Unique one-body position operator for periodic systems. Physical Review B, 2022, 105, .	3.2	6
105	A surface hopping study of energy transfer in Na + Cdâ^—* collisions. Chemical Physics Letters, 1996, 255, 65-70.	2.6	5
106	FRODO: a MuPAD program to calculate matrix elements between contracted wavefunctions. Computer Physics Communications, 2005, 171, 63-68.	7.5	5
107	The localization spread and polarizability of rings and periodic chains. Journal of Chemical Physics, 2021, 155, 124107.	3.0	4
108	A priori complete active space self consistent field localized orbitals: an application on linear polyenes. Molecular Physics, 2006, 104, 691-700.	1.7	3

#	Article	IF	Citations
109	Some Useful Odds and Ends From the n-Electron Valence State Perturbation Theory. Journal of Physical Chemistry A, 2014, 118, 6435-6439.	2.5	3
110	Complexation of transition metal cations (Sc+, Fe+, Cu+) by one cyanide radical ##dedicated to Professor Del Re. Advances in Quantum Chemistry, 2000, 36, 271-282.	0.8	2
111	The Calculation of the Correlation Energy in Ground and Excited States: the nâ€“Electron Valence State Perturbation Theory Approach. AIP Conference Proceedings, 2007, , .	0.4	2
112	Temperature and composition dependence of the Soret coefficient in Lennard-Jones mixtures presenting consolute critical phenomena. Journal of Chemical Physics, 2010, 132, 124512.	3.0	2
113	Dependence of the Population on the Temperature in the Boltzmann Distribution: A Simple Relation Involving the Average Energy. Journal of Chemical Education, 2013, 90, 1639-1644.	2.3	2
114	Kmonodim, a Program for the Numerical Solution of the One-Dimensional SchÃ¶dinger Equation. Journal of Chemical Education, 2005, 82, 795.	2.3	1
115	Temperature and composition dependence of the Soret coefficient in Lennard-Jones mixtures presenting evaporation/condensation phase transition. Journal of Chemical Physics, 2011, 134, 114512.	3.0	1
116	Automated evaluation of matrix elements between contracted wavefunctions: A Mathematica version of the FRODO program. Computer Physics Communications, 2013, 184, 443-444.	7.5	0