Celestino Angeli

List of Publications by Citations

115 papers	6,822 citations	33 h-index	81 g-index
119 ext. papers	7,649 ext. citations	3.4 avg, IF	5.64 L-index

#	Paper	IF	Citations
115	Introduction of n-electron valence states for multireference perturbation theory. *Journal of Chemical Physics*, **2001**, 114, 10252-10264	3.9	1069
114	The Dalton quantum chemistry program system. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 269-284	7.9	956
113	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	3.9	720
112	N-electron valence state perturbation theory: a fast implementation of the strongly contracted variant. *Chemical Physics Letters*, **2001**, 350, 297-305	2.5	523
111	OpenMolcas: From Source Code to Insight. *Journal of Chemical Theory and Computation*, **2019**, 15, 5925-5964	5.4	310
110	A quasidegenerate formulation of the second order n-electron valence state perturbation theory approach. *Journal of Chemical Physics*, **2004**, 121, 4043-9	3.9	238
109	New perspectives in multireference perturbation theory: the n-electron valence state approach. *Theoretical Chemistry Accounts*, **2007**, 117, 743-754	1.9	216
108	Third-order multireference perturbation theory: the n-electron valence state perturbation-theory approach. *Journal of Chemical Physics*, **2006**, 124, 054108	3.9	133
107	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, 3074-84	6.4	132
106	Dynamic Electron Correlation Effects on the Ground State Potential Energy Surface of a Retinal Chromophore Model. *Journal of Chemical Theory and Computation*, **2012**, 8, 4069-80	6.4	127
105	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	3.9	101
104	On the nature of the pi --> pi* ionic excited states: the V state of ethene as a prototype. *Journal of Computational Chemistry*, **2009**, 30, 1319-33	3.5	95
103	On the applicability of multireference second-order perturbation theory to study weak magnetic coupling in molecular complexes. *Journal of Computational Chemistry*, **2008**, 29, 994-1003	3.5	79
102	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, 4495-506	6.4	76
101	Multireference Perturbation Theory with Cholesky Decomposition for the Density Matrix Renormalization Group. *Journal of Chemical Theory and Computation*, **2017**, 13, 451-459	6.4	73
100	A novel perturbation-based complete active space self-consistent-field algorithm: Application to the direct calculation of localized orbitals. *Journal of Chemical Physics*, **2002**, 117, 10525-10533	3.9	59
99	Multireference perturbation CI I. Extrapolation procedures with CAS or selected zero-order spaces. *Theoretical Chemistry Accounts*, **1997**, 98, 57-63	1.9	54

98	Bond electron pair: its relevance and analysis from the quantum chemistry point of view. *Journal of Computational Chemistry*, **2007**, 28, 35-50	3.5	54
97	Multireference perturbation CI II. Selection of the zero-order space. *Theoretical Chemistry Accounts*, **1997**, 98, 117-128	1.9	52
96	Multireference perturbation configuration interaction V. Third-order energy contributions in the Møller–Plesset and Epstein–Nesbet partitions. *Theoretical Chemistry Accounts*, **2002**, 107, 313-317	1.9	52
95	Metal-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, 11916-34	5.1	50
94	Excitation energies of retinal chromophores: critical role of the structural model. *Physical Chemistry Chemical Physics*, **2012**, 14, 11015-20	3.6	47
93	The lowest singlet states of octatetraene revisited. *Journal of Chemical Physics*, **2011**, 134, 184302	3.9	46
92	Calibration of the n-electron valence state perturbation theory approach. *Journal of Chemical Physics*, **2004**, 120, 4619-25	3.9	46
91	On the Relative Merits of Non-Orthogonal and Orthogonal Valence Bond Methods Illustrated on the Hydrogen Molecule. *Journal of Chemical Education*, **2008**, 85, 150	2.4	42
90	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	4.9	41
89	A convenient decontraction procedure of internally contracted state-specific multireference algorithms. *Journal of Chemical Physics*, **2006**, 124, 234109	3.9	39
88	On a mixed Møller–Plesset Epstein–Nesbet partition of the Hamiltonian to be used in multireference perturbation configuration interaction. *Chemical Physics Letters*, **2000**, 317, 472-480	2.5	39
87	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	3.9	38
86	Beryllium dimer: a bond based on non-dynamical correlation. *Journal of Physical Chemistry A*, **2014**, 118, 6664-73	2.8	36
85	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, 4014-24	6.4	34
84	The use of local orbitals in multireference calculations. *Molecular Physics*, **2003**, 101, 1389-1398	1.7	33
83	An application of second-order n-electron valence state perturbation theory to the calculation of excited states. *Theoretical Chemistry Accounts*, **2004**, 111, 352-357	1.9	33
82	The problem of interoperability: A common data format for quantum chemistry codes. *International Journal of Quantum Chemistry*, **2007**, 107, 2082-2091	2.1	31
81	Analysis of the magnetic coupling in nitroxide organic biradicals. *Theoretical Chemistry Accounts*, **2011**, 128, 505-519	1.9	30

80	The effect of thermodiffusion on the stability of a salinity gradient solar pond. *International Journal of Heat and Mass Transfer*, **2005**, 48, 4633-4639	4.9	30
79	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	3.9	29
78	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	3.9	29
77	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	2.5	28
76	Metal-to-metal charge-transfer transitions: reliable excitation energies from ab initio calculations. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	26
75	An ab initio multireference perturbation theory study on the manganese dimer. *Journal of Chemical Physics*, **2008**, 128, 244317	3.9	26
74	X-ray absorption and resonant Auger spectroscopy of O2 in the vicinity of the O 1s-->sigma* resonance: experiment and theory. *Journal of Chemical Physics*, **2008**, 128, 064304	3.9	26
73	FORTRAN interface for code interoperability in quantum chemistry: the Q5Cost library. *Journal of Chemical Information and Modeling*, **2007**, 47, 1271-7	6.1	26
72	On the controversial nature of the 1 1B(u) and 2 1B(u) states of trans-stilbene: the n-electron valence state perturbation theory approach. *Journal of Chemical Physics*, **2009**, 130, 174307	3.9	25
71	On the competition between the inversion and rotation mechanisms in the cis-trans thermal isomerization of diazene. *Chemical Physics Letters*, **1996**, 259, 276-282	2.5	25
70	Charge-displacement analysis for excited states. *Journal of Chemical Physics*, **2014**, 140, 054110	3.9	24
69	Dynamical photoionization observables of the CS molecule: the role of electron correlation. *Journal of Chemical Physics*, **2014**, 140, 204304	3.9	24
68	Extending the active space in multireference configuration interaction calculations of magnetic coupling constants. *Theoretical Chemistry Accounts*, **2010**, 126, 185-196	1.9	24
67	A computational study of salt diffusion and heat extraction in solar pond plants. *Solar Energy*, **2006**, 80, 1498-1508	6.8	23
66	Threshold Photoionization Study of Fe(CO)5 versus ab Initio Calculations. *Journal of Physical Chemistry A*, **1997**, 101, 7907-7913	2.8	22
65	Quasi-bond orbitals from maximum-localization hybrids for ab initio CI calculations. *Chemical Physics Letters*, **1995**, 233, 102-110	2.5	22
64	Magnetic behaviour vs. structural changes in an isomeric series of binuclear copper(II) complexes: an experimental and theoretical study. *New Journal of Chemistry*, **2014**, 38, 574-583	3.6	21
63	The electronic structure of Ullman's biradicals: an orthogonal valence bond interpretation. *Physical Chemistry Chemical Physics*, **2011**, 13, 14617-28	3.6	21

62	Electronic structure investigation of the evanescent AtO(+) ion. *Physical Chemistry Chemical Physics*, **2014**, 16, 9238-48	3.6	20
61	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	3.9	20
60	A multireference perturbation theory study on the Fe2 molecule: in quest of the ground state. *Molecular Physics*, **2011**, 109, 1503-1509	1.7	20
59	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	20
58	A multireference perturbation theory study on the vertical electronic spectrum of thiophene. *Theoretical Chemistry Accounts*, **2007**, 118, 35-46	1.9	20
57	Multiple complete active space self-consistent field solutions. *Molecular Physics*, **2003**, 101, 1937-1944	1.7	20
56	Constant-atomic-final-state filtering of dissociative states in the O1s-->sigma* core excitation in O2. *Journal of Chemical Physics*, **2005**, 123, 64314	3.9	20
55	On the Maxwell-Stefan approach to diffusion: a general resolution in the transient regime for one-dimensional systems. *Journal of Physical Chemistry B*, **2010**, 114, 151-64	3.4	19
54	O 1s --> sigma* resonance in O2: inadequacy of only two exchange-split components. *Physical Review Letters*, **2002**, 88, 243002	7.4	19
53	Metal-ligand delocalization and spin density in the CuCl2 and [CuCl4](2-) molecules: Some insights from wave function theory. *Journal of Chemical Physics*, **2015**, 143, 124305	3.9	18
52	Multireference perturbation CI III. Fast evaluation of the one-particle density matrix. *Theoretical Chemistry Accounts*, **1998**, 100, 324-328	1.9	18
51	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	2.5	18
50	Code interoperability and standard data formats in quantum chemistry and quantum dynamics: The Q5/D5Cost data model. *Journal of Computational Chemistry*, **2014**, 35, 611-21	3.5	17
49	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		17
48	Improving the calculation of magnetic coupling constants in MRPT methods. *Journal of Computational Chemistry*, **2014**, 35, 1665-71	3.5	16
47	Aromaticity: an ab initio evaluation of the properly cyclic delocalization energy and the pi-delocalization energy distortivity of benzene. *Journal of Physical Chemistry A*, **2008**, 112, 11481-6	2.8	16
46	A perturbation-based super-CI approach for the orbital optimization of a CASSCF wave function. *Journal of Computational Chemistry*, **2019**, 40, 1463-1470	3.5	15
45	Highly efficient perturbative + variational strategy based on orthogonal valence bond theory for the evaluation of magnetic coupling constants. Application to the trinuclear Cu(ii) site of multicopper oxidases. *Physical Chemistry Chemical Physics*, **2016**, 18, 18365-80	3.6	15

44	Non-orthogonal and orthogonal valence bond wavefunctions in the hydrogen molecule: the diabatic view. *Molecular Physics*, **2013**, 111, 1069-1077	1.7	15
43	Behavior of the Position-Spread Tensor in Diatomic Systems. *Journal of Chemical Theory and Computation*, **2013**, 9, 5286-95	6.4	15
42	The Effect of the Basis-Set Superposition Error on the Calculation of Dispersion Interactions: A Test Study on the Neon Dimer. *Journal of Chemical Theory and Computation*, **2007**, 3, 477-85	6.4	15
41	Photoionization of furan from the ground and excited electronic states. *Journal of Chemical Physics*, **2016**, 144, 084307	3.9	15
40	Can the second order multireference perturbation theory be considered a reliable tool to study mixed-valence compounds?. *Journal of Chemical Physics*, **2008**, 128, 174102	3.9	14
39	Caging 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	2.3	13
38	A theoretical study of Be(N) linear chains: variational and perturbative approaches. *Journal of Chemical Physics*, **2009**, 131, 034309	3.9	13
37	An analysis of the dynamic polarization in the V state of ethene. *International Journal of Quantum Chemistry*, **2010**, 110, NA-NA	2.1	13
36	Multireference perturbation CI IV. Selection procedure for one-electron properties. *Theoretical Chemistry Accounts*, **2001**, 105, 259-264	1.9	13
35	Electronic reorganization triggered by electron transfer: the intervalence charge transfer of a Fe+/Fe+ bimetallic complex. *Journal of Computational Chemistry*, **2015**, 36, 861-9	3.5	12
34	Assessment of multireference perturbation methods for chemical reaction barrier heights. *Journal of Physical Chemistry A*, **2015**, 119, 5490-5	2.8	12
33	Developments in the n-electron valence state perturbation theory. *International Journal of Quantum Chemistry*, **2006**, 106, 686-691	2.1	12
32	Quasi-diabatic and adiabatic states and potential energy curves for Na?Cd collisions and excimer formation. *Chemical Physics*, **1996**, 204, 57-64	2.3	12
31	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	3.9	11
30	A Simple Approximate Perturbation Approach to Quasi-degenerate Systems. *Theoretical Chemistry Accounts*, **2006**, 116, 434-439	1.9	11
29	Common Format for Quantum Chemistry Interoperability: Q5Cost Format and Library. *Lecture Notes in Computer Science*, **2008**, 1094-1107	0.9	11
28	A multireference n-electron Valence State Perturbation Theory study of the electronic spectrum of s-tetrazine. *Theoretical Chemistry Accounts*, **2009**, 123, 287-298	1.9	10
27	Optical absorption spectrum of the N3 solar cell sensitizer by second-order multireference perturbation theory. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	10

26	Geometry optimization within a localized CAS-SCF approach. *Chemical Physics Letters*, **2003**, 371, 49-55	2.5	9
25	Local orbitals for quasi-degenerate systems. *Computational and Theoretical Chemistry*, **2004**, 709, 1-10		8
24	Spin density and orbital optimization in open shell systems: A rational and computationally efficient proposal. *Journal of Chemical Physics*, **2016**, 144, 104104	3.9	8
23	Strongly localized approaches for delocalized systems. I. Ground state of linear polyenes. *Computational and Theoretical Chemistry*, **2017**, 1116, 102-111	2	7
22	Computer assisted generation of the matrix elements between contracted wavefunctions in a Complete Active Space scheme. *Computer Physics Communications*, **2005**, 166, 53-57	4.2	7
21	Physical Interpretation of Koopmans' Theorem: A Criticism of the Current Didactic Presentation. *Journal of Chemical Education*, **1998**, 75, 1494	2.4	7
20	Application of a charge-averaged second order multireference perturbation theory strategy to the study of a model Mixed-Valence compound. *Computational and Theoretical Chemistry*, **2009**, 896, 12-17		6
19	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	3.9	6
18	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	5.4	5
17	The Intriguing Case of the One-Photon and Two-Photon Absorption of a Prototypical Symmetric Squaraine: Comparison of TDDFT and Wave-Function Methods. *ChemPhotoChem*, **2019**, 3, 778-793	3.3	5
16	The Møller-Plesset perturbation revisited: origin of high-order divergences. *Molecular Physics*, **2013**, 111, 1092-1099	1.7	5
15	FRODO: a MuPAD program to calculate matrix elements between contracted wavefunctions. *Computer Physics Communications*, **2005**, 171, 63-68	4.2	5
14	The Spin-Partitioned Total-Position Spread Tensor: An Application To Diatomic Molecules. *Journal of Physical Chemistry A*, **2016**, 120, 5230-8	2.8	5
13	Transient Diffusion within Spherical Particles: Numerical Resolution of the Maxwell-Stefan Formulation. *Industrial & Engineering Chemistry Research*, **2010**, 49, 5654-5660	3.9	4
12	A surface hopping study of energy transfer in Na + Cd** collisions. *Chemical Physics Letters*, **1996**, 255, 65-70	2.5	4
11	OpenMolcas: From Source Code to Insight		4
10	Some useful odds and ends from the n-electron valence state perturbation theory. *Journal of Physical Chemistry A*, **2014**, 118, 6435-9	2.8	3
9	A priori complete active space self consistent field localized orbitals: an application on linear polyenes. *Molecular Physics*, **2006**, 104, 691-700	1.7	3

8	The "Fermi hole" and the correlation introduced by the symmetrization or the anti-symmetrization of the wave function. *Journal of Chemical Physics*, **2016**, 145, 124114	3.9	3
7	Temperature and composition dependence of the Soret coefficient in Lennard-Jones mixtures presenting consolute critical phenomena. *Journal of Chemical Physics*, **2010**, 132, 124512	3.9	2
6	Complexation of transition metal cations (Sc+, Fe+, Cu+) by one cyanide radical. *Advances in Quantum Chemistry*, **2000**, 36, 271-282	1.4	2
5	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	2.4	1
4	The Calculation of the Correlation Energy in Ground and Excited States: the n-Electron Valence State Perturbation Theory Approach. *AIP Conference Proceedings*, **2007**,	0	1
3	Kmonodim, a Program for the Numerical Solution of the One-Dimensional Schrödinger Equation. *Journal of Chemical Education*, **2005**, 82, 795	2.4	1
2	The localization spread and polarizability of rings and periodic chains. *Journal of Chemical Physics*, **2021**, 155, 124107	3.9	1
1	Temperature and composition dependence of the Soret coefficient in Lennard-Jones mixtures presenting evaporation/condensation phase transition. *Journal of Chemical Physics*, **2011**, 134, 114512	3.9	0