

Celestino Angeli

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	The localization spread and polarizability of rings and periodic chains. <i>Journal of Chemical Physics</i> , 2021 , 155, 124107	3.9	1
114	OpenMolcas: From Source Code to Insight. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 5925-5964	3.4	310
113	The Intriguing Case of the One-Photon and Two-Photon Absorption of a Prototypical Symmetric Squaraine: Comparison of TDDFT and Wave-Function Methods. <i>ChemPhotoChem</i> , 2019 , 3, 778-793	3.3	5
112	A perturbation-based super-CI approach for the orbital optimization of a CASSCF wave function. <i>Journal of Computational Chemistry</i> , 2019 , 40, 1463-1470	3.5	15
111	Computation of the Isotropic Hyperfine Coupling Constant: Efficiency and Insights from a New Approach Based on Wave Function Theory. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 475-487	6.4	5
110	Strongly localized approaches for delocalized systems. I. Ground state of linear polyenes. <i>Computational and Theoretical Chemistry</i> , 2017 , 1116, 102-111	2	7
109	Multireference Perturbation Theory with Cholesky Decomposition for the Density Matrix Renormalization Group. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 451-459	6.4	73
108	A Jeziorski-Monkhorst fully uncontracted multi-reference perturbative treatment. I. Principles, second-order versions, and tests on ground state potential energy curves. <i>Journal of Chemical Physics</i> , 2017 , 146, 224108	3.9	20
107	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. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 18365-80	3.6	15
106	Spin density and orbital optimization in open shell systems: A rational and computationally efficient proposal. <i>Journal of Chemical Physics</i> , 2016 , 144, 104104	3.9	8
105	Photoionization of furan from the ground and excited electronic states. <i>Journal of Chemical Physics</i> , 2016 , 144, 084307	3.9	15
104	The "Fermi hole" and the correlation introduced by the symmetrization or the anti-symmetrization of the wave function. <i>Journal of Chemical Physics</i> , 2016 , 145, 124114	3.9	3
103	The Spin-Partitioned Total-Position Spread Tensor: An Application To Diatomic Molecules. <i>Journal of Physical Chemistry A</i> , 2016 , 120, 5230-8	2.8	5
102	Optical absorption spectrum of the N3 solar cell sensitizer by second-order multireference perturbation theory. <i>Theoretical Chemistry Accounts</i> , 2016 , 135, 1	1.9	10
101	Metal-ligand delocalization and spin density in the CuCl ₂ and [CuCl ₄] ²⁻ molecules: Some insights from wave function theory. <i>Journal of Chemical Physics</i> , 2015 , 143, 124305	3.9	18
100	Electronic reorganization triggered by electron transfer: the intervalence charge transfer of a Fe ^{II} /Fe ^{III} bimetallic complex. <i>Journal of Computational Chemistry</i> , 2015 , 36, 861-9	3.5	12
99	Metal-Metal Interactions in Trinuclear Copper(II) Complexes [Cu ₃ (RCOO) ₄ (H ₂ TEA) ₂] and Binuclear [Cu ₂ (RCOO) ₂ (H ₂ TEA) ₂]. Syntheses and Combined Structural, Magnetic, High-Field Electron Paramagnetic Resonance, and Theoretical Studies. <i>Inorganic Chemistry</i> , 2015 , 54, 11916-34	5.1	50

98	Assessment of multireference perturbation methods for chemical reaction barrier heights. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 5490-5	2.8	12
97	Magnetic behaviour vs. structural changes in an isomeric series of binuclear copper(II) complexes: an experimental and theoretical study. <i>New Journal of Chemistry</i> , 2014 , 38, 574-583	3.6	21
96	The Dalton quantum chemistry program system. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2014 , 4, 269-284	7.9	956
95	Electronic structure investigation of the evanescent AtO(+) ion. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 9238-48	3.6	20
94	Some useful odds and ends from the n-electron valence state perturbation theory. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 6435-9	2.8	3
93	Density Relaxation in Time-Dependent Density Functional Theory: Combining Relaxed Density Natural Orbitals and Multireference Perturbation Theories for an Improved Description of Excited States. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 4014-24	6.4	34
92	Shape of Multireference, Equation-of-Motion Coupled-Cluster, and Density Functional Theory Potential Energy Surfaces at a Conical Intersection. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 3074-84	6.4	132
91	Beryllium dimer: a bond based on non-dynamical correlation. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 6664-73	2.8	36
90	Charge-displacement analysis for excited states. <i>Journal of Chemical Physics</i> , 2014 , 140, 054110	3.9	24
89	Code interoperability and standard data formats in quantum chemistry and quantum dynamics: The Q5/D5Cost data model. <i>Journal of Computational Chemistry</i> , 2014 , 35, 611-21	3.5	17
88	Improving the calculation of magnetic coupling constants in MRPT methods. <i>Journal of Computational Chemistry</i> , 2014 , 35, 1665-71	3.5	16
87	Dynamical photoionization observables of the CS molecule: the role of electron correlation. <i>Journal of Chemical Physics</i> , 2014 , 140, 204304	3.9	24
86	The Müller-Plesset perturbation revisited: origin of high-order divergences. <i>Molecular Physics</i> , 2013 , 111, 1092-1099	1.7	5
85	Mapping the Excited State Potential Energy Surface of a Retinal Chromophore Model with Multireference and Equation-of-Motion Coupled-Cluster Methods. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 4495-506	6.4	76
84	Dependence of the Population on the Temperature in the Boltzmann Distribution: A Simple Relation Involving the Average Energy. <i>Journal of Chemical Education</i> , 2013 , 90, 1639-1644	2.4	1
83	Non-orthogonal and orthogonal valence bond wavefunctions in the hydrogen molecule: the diabatic view. <i>Molecular Physics</i> , 2013 , 111, 1069-1077	1.7	15
82	Behavior of the Position-Spread Tensor in Diatomic Systems. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 5286-95	6.4	15
81	The localization tensor for the H ₂ molecule: closed formulae for the Heitler-London and related wavefunctions and comparison with full configuration interaction. <i>Journal of Chemical Physics</i> , 2013 , 138, 054314	3.9	11

80	Tagging Anions through Crystal Engineering to Avoid Polymerization: Structural, Conformational and Theoretical Investigations of New Halocadmate [Cd ₂ X ₇] ₃ Anions (X = Cl/Br). <i>European Journal of Inorganic Chemistry</i> , 2012 , 2012, 1195-1203	2.3	13
79	Excitation energies of retinal chromophores: critical role of the structural model. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 11015-20	3.6	47
78	The role of the magnetic orbitals in the calculation of the magnetic coupling constants from multireference perturbation theory methods. <i>Journal of Chemical Physics</i> , 2012 , 137, 034104	3.9	38
77	Dynamic Electron Correlation Effects on the Ground State Potential Energy Surface of a Retinal Chromophore Model. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 4069-80	6.4	127
76	Metal-to-metal charge-transfer transitions: reliable excitation energies from ab initio calculations. <i>Theoretical Chemistry Accounts</i> , 2012 , 131, 1	1.9	26
75	A comparison of various approaches in internally contracted multireference configuration interaction: the carbon dimer as a test case. <i>Molecular Physics</i> , 2012 , 110, 2963-2968	1.7	20
74	The electronic structure of Ullman's biradicals: an orthogonal valence bond interpretation. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 14617-28	3.6	21
73	Analysis of the magnetic coupling in nitroxide organic biradicals. <i>Theoretical Chemistry Accounts</i> , 2011 , 128, 505-519	1.9	30
72	A multireference perturbation theory study on the Fe ₂ molecule: in quest of the ground state. <i>Molecular Physics</i> , 2011 , 109, 1503-1509	1.7	20
71	The lowest singlet states of octatetraene revisited. <i>Journal of Chemical Physics</i> , 2011 , 134, 184302	3.9	46
70	Temperature and composition dependence of the Soret coefficient in Lennard-Jones mixtures presenting evaporation/condensation phase transition. <i>Journal of Chemical Physics</i> , 2011 , 134, 114512	3.9	0
69	Transient Diffusion within Spherical Particles: Numerical Resolution of the Maxwell-Stefan Formulation. <i>Industrial & Engineering Chemistry Research</i> , 2010 , 49, 5654-5660	3.9	4
68	On the Maxwell-Stefan approach to diffusion: a general resolution in the transient regime for one-dimensional systems. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 151-64	3.4	19
67	Temperature and composition dependence of the Soret coefficient in Lennard-Jones mixtures presenting consolute critical phenomena. <i>Journal of Chemical Physics</i> , 2010 , 132, 124512	3.9	2
66	Extending the active space in multireference configuration interaction calculations of magnetic coupling constants. <i>Theoretical Chemistry Accounts</i> , 2010 , 126, 185-196	1.9	24
65	An analysis of the dynamic polarization in the V state of ethene. <i>International Journal of Quantum Chemistry</i> , 2010 , 110, NA-NA	2.1	13
64	Analysis of the magnetic coupling in binuclear systems. III. The role of the ligand to metal charge transfer excitations revisited. <i>Journal of Chemical Physics</i> , 2009 , 131, 044327	3.9	101
63	On the nature of the pi → pi* ionic excited states: the V state of ethene as a prototype. <i>Journal of Computational Chemistry</i> , 2009 , 30, 1319-33	3.5	95

62	A multireference n-electron Valence State Perturbation Theory study of the electronic spectrum of s-tetrazine. <i>Theoretical Chemistry Accounts</i> , 2009 , 123, 287-298	1.9	10
61	Application of a charge-averaged second order multireference perturbation theory strategy to the study of a model Mixed-Valence compound. <i>Computational and Theoretical Chemistry</i> , 2009 , 896, 12-17		6
60	A theoretical study of Be(N) linear chains: variational and perturbative approaches. <i>Journal of Chemical Physics</i> , 2009 , 131, 034309	3.9	13
59	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. <i>Journal of Chemical Physics</i> , 2009 , 130, 174307	3.9	25
58	An ab initio multireference perturbation theory study on the manganese dimer. <i>Journal of Chemical Physics</i> , 2008 , 128, 244317	3.9	26
57	On the Relative Merits of Non-Orthogonal and Orthogonal Valence Bond Methods Illustrated on the Hydrogen Molecule. <i>Journal of Chemical Education</i> , 2008 , 85, 150	2.4	42
56	Aromaticity: an ab initio evaluation of the properly cyclic delocalization energy and the pi-delocalization energy distortivity of benzene. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 11481-6	2.8	16
55	Can the second order multireference perturbation theory be considered a reliable tool to study mixed-valence compounds?. <i>Journal of Chemical Physics</i> , 2008 , 128, 174102	3.9	14
54	X-ray absorption and resonant Auger spectroscopy of O2 in the vicinity of the O 1s-->sigma* resonance: experiment and theory. <i>Journal of Chemical Physics</i> , 2008 , 128, 064304	3.9	26
53	Influence of the interaction potential and of the temperature on the thermodiffusion (Soret) coefficient in a model system. <i>Journal of Chemical Physics</i> , 2008 , 128, 054507	3.9	6
52	On the applicability of multireference second-order perturbation theory to study weak magnetic coupling in molecular complexes. <i>Journal of Computational Chemistry</i> , 2008 , 29, 994-1003	3.5	79
51	Common Format for Quantum Chemistry Interoperability: Q5Cost Format and Library. <i>Lecture Notes in Computer Science</i> , 2008 , 1094-1107	0.9	11
50	FORTTRAN interface for code interoperability in quantum chemistry: the Q5Cost library. <i>Journal of Chemical Information and Modeling</i> , 2007 , 47, 1271-7	6.1	26
49	Bond electron pair: its relevance and analysis from the quantum chemistry point of view. <i>Journal of Computational Chemistry</i> , 2007 , 28, 35-50	3.5	54
48	The problem of interoperability: A common data format for quantum chemistry codes. <i>International Journal of Quantum Chemistry</i> , 2007 , 107, 2082-2091	2.1	31
47	New perspectives in multireference perturbation theory: the n-electron valence state approach. <i>Theoretical Chemistry Accounts</i> , 2007 , 117, 743-754	1.9	216
46	A multireference perturbation theory study on the vertical electronic spectrum of thiophene. <i>Theoretical Chemistry Accounts</i> , 2007 , 118, 35-46	1.9	20
45	Ground states of the Mo2, W2, and CrMo molecules: a second and third order multireference perturbation theory study. <i>Journal of Chemical Physics</i> , 2007 , 127, 074306	3.9	29

44	The Calculation of the Correlation Energy in Ground and Excited States: the n-Electron Valence State Perturbation Theory Approach. <i>AIP Conference Proceedings</i> , 2007 ,	0	1
43	The Effect of the Basis-Set Superposition Error on the Calculation of Dispersion Interactions: A Test Study on the Neon Dimer. <i>Journal of Chemical Theory and Computation</i> , 2007 , 3, 477-85	6.4	15
42	A Simple Approximate Perturbation Approach to Quasi-degenerate Systems. <i>Theoretical Chemistry Accounts</i> , 2006 , 116, 434-439	1.9	11
41	Third-order multireference perturbation theory: the n-electron valence state perturbation-theory approach. <i>Journal of Chemical Physics</i> , 2006 , 124, 054108	3.9	133
40	A convenient decontraction procedure of internally contracted state-specific multireference algorithms. <i>Journal of Chemical Physics</i> , 2006 , 124, 234109	3.9	39
39	A priori complete active space self consistent field localized orbitals: an application on linear polyenes. <i>Molecular Physics</i> , 2006 , 104, 691-700	1.7	3
38	Developments in the n-electron valence state perturbation theory. <i>International Journal of Quantum Chemistry</i> , 2006 , 106, 686-691	2.1	12
37	The vertical electronic spectrum of pyrrole: A second and third order n-electron valence state perturbation theory study. <i>Chemical Physics Letters</i> , 2006 , 422, 522-528	2.5	28
36	An application of second and third-order n-electron valence state perturbation theory to the calculation of the vertical electronic spectrum of furan. <i>Chemical Physics Letters</i> , 2006 , 426, 445-451	2.5	18
35	A computational study of salt diffusion and heat extraction in solar pond plants. <i>Solar Energy</i> , 2006 , 80, 1498-1508	6.8	23
34	Kmonodim, a Program for the Numerical Solution of the One-Dimensional Schrödinger Equation. <i>Journal of Chemical Education</i> , 2005 , 82, 795	2.4	1
33	The effect of thermodiffusion on the stability of a salinity gradient solar pond. <i>International Journal of Heat and Mass Transfer</i> , 2005 , 48, 4633-4639	4.9	30
32	A CASSCF theoretical study of the vibrational frequencies and structure of formaldehyde, acetaldehyde and acetone valence excited states. <i>Computational and Theoretical Chemistry</i> , 2005 , 718, 55-69		17
31	Computer assisted generation of the matrix elements between contracted wavefunctions in a Complete Active Space scheme. <i>Computer Physics Communications</i> , 2005 , 166, 53-57	4.2	7
30	FRODO: a MuPAD program to calculate matrix elements between contracted wavefunctions. <i>Computer Physics Communications</i> , 2005 , 171, 63-68	4.2	5
29	Ab initio n-electron valence state perturbation theory study of the adiabatic transitions in carbonyl molecules: formaldehyde, acetaldehyde, and acetone. <i>Journal of Chemical Physics</i> , 2005 , 122, 114304	3.9	29
28	Constant-atomic-final-state filtering of dissociative states in the O1s-->sigma* core excitation in O2. <i>Journal of Chemical Physics</i> , 2005 , 123, 64314	3.9	20
27	A quasidegenerate formulation of the second order n-electron valence state perturbation theory approach. <i>Journal of Chemical Physics</i> , 2004 , 121, 4043-9	3.9	238

26	Local orbitals for quasi-degenerate systems. <i>Computational and Theoretical Chemistry</i> , 2004 , 709, 1-10		8
25	A one-dimensional numerical study of the salt diffusion in a salinity-gradient solar pond. <i>International Journal of Heat and Mass Transfer</i> , 2004 , 47, 1-10	4.9	41
24	Calibration of the n-electron valence state perturbation theory approach. <i>Journal of Chemical Physics</i> , 2004 , 120, 4619-25	3.9	46
23	An application of second-order n-electron valence state perturbation theory to the calculation of excited states. <i>Theoretical Chemistry Accounts</i> , 2004 , 111, 352-357	1.9	33
22	Geometry optimization within a localized CAS-SCF approach. <i>Chemical Physics Letters</i> , 2003 , 371, 49-55	2.5	9
21	The use of local orbitals in multireference calculations. <i>Molecular Physics</i> , 2003 , 101, 1389-1398	1.7	33
20	Multiple complete active space self-consistent field solutions. <i>Molecular Physics</i> , 2003 , 101, 1937-1944	1.7	20
19	Multireference perturbation configuration interaction V. Third-order energy contributions in the Møller-Plesset and Epstein-Nesbet partitions. <i>Theoretical Chemistry Accounts</i> , 2002 , 107, 313-317	1.9	52
18	O 1s → sigma* resonance in O ₂ : inadequacy of only two exchange-split components. <i>Physical Review Letters</i> , 2002 , 88, 243002	7.4	19
17	n-electron valence state perturbation theory: A spinless formulation and an efficient implementation of the strongly contracted and of the partially contracted variants. <i>Journal of Chemical Physics</i> , 2002 , 117, 9138-9153	3.9	720
16	A novel perturbation-based complete active space self-consistent-field algorithm: Application to the direct calculation of localized orbitals. <i>Journal of Chemical Physics</i> , 2002 , 117, 10525-10533	3.9	59
15	Multireference perturbation CI IV. Selection procedure for one-electron properties. <i>Theoretical Chemistry Accounts</i> , 2001 , 105, 259-264	1.9	13
14	N-electron valence state perturbation theory: a fast implementation of the strongly contracted variant. <i>Chemical Physics Letters</i> , 2001 , 350, 297-305	2.5	523
13	Introduction of n-electron valence states for multireference perturbation theory. <i>Journal of Chemical Physics</i> , 2001 , 114, 10252-10264	3.9	1069
12	Complexation of transition metal cations (Sc ⁺ , Fe ⁺ , Cu ⁺) by one cyanide radical. <i>Advances in Quantum Chemistry</i> , 2000 , 36, 271-282	1.4	2
11	On a mixed Møller-Plesset Epstein-Nesbet partition of the Hamiltonian to be used in multireference perturbation configuration interaction. <i>Chemical Physics Letters</i> , 2000 , 317, 472-480	2.5	39
10	Multireference perturbation CI III. Fast evaluation of the one-particle density matrix. <i>Theoretical Chemistry Accounts</i> , 1998 , 100, 324-328	1.9	18
9	Physical Interpretation of Koopmans' Theorem: A Criticism of the Current Didactic Presentation. <i>Journal of Chemical Education</i> , 1998 , 75, 1494	2.4	7

8	Threshold Photoionization Study of Fe(CO) ₅ versus ab Initio Calculations. <i>Journal of Physical Chemistry A</i> , 1997 , 101, 7907-7913	2.8	22
7	Multireference perturbation CI I. Extrapolation procedures with CAS or selected zero-order spaces. <i>Theoretical Chemistry Accounts</i> , 1997 , 98, 57-63	1.9	54
6	Multireference perturbation CI II. Selection of the zero-order space. <i>Theoretical Chemistry Accounts</i> , 1997 , 98, 117-128	1.9	52
5	Quasi-diabatic and adiabatic states and potential energy curves for Na?Cd collisions and excimer formation. <i>Chemical Physics</i> , 1996 , 204, 57-64	2.3	12
4	On the competition between the inversion and rotation mechanisms in the cis-trans thermal isomerization of diazene. <i>Chemical Physics Letters</i> , 1996 , 259, 276-282	2.5	25
3	A surface hopping study of energy transfer in Na + Cd** collisions. <i>Chemical Physics Letters</i> , 1996 , 255, 65-70	2.5	4
2	Quasi-bond orbitals from maximum-localization hybrids for ab initio CI calculations. <i>Chemical Physics Letters</i> , 1995 , 233, 102-110	2.5	22
1	OpenMolcas: From Source Code to Insight		4