Renzo Cimiraglia

List of Publications by Year
in descending order

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84 papers	5,522 citations	159585 30 h-index	76900 74 g-index
84 all docs	84 docs citations	84 times ranked	4052 citing authors

#	Article	IF	Citations
1	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	14.6	1,166
2	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
3	N-electron valence state perturbation theory: a fast implementation of the strongly contracted variant. Chemical Physics Letters, 2001, 350, 297-305.	2.6	689
4	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
5	New perspectives in multireference perturbation theory: the n-electron valence state approach. Theoretical Chemistry Accounts, 2007, 117, 743-754.	1.4	238
6	Third-order multireference perturbation theory: The n-electron valence state perturbation-theory approach. Journal of Chemical Physics, 2006, 124, 054108.	3.0	151
7	Recent advances in multireference second order perturbation CI: The CIPSI method revisited. Journal of Computational Chemistry, 1987, 8, 39-47.	3.3	117
8	Second order perturbation correction to CI energies by use of diagrammatic techniques: An improvement to the CIPSI algorithm. Journal of Chemical Physics, 1985, 83, 1746-1749.	3.0	104
9	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
10	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
11	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
12	Merging multireference perturbation and density-functional theories by means of range separation: Potential curves for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Be</mml:mi><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>,<mml: xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Mg</mml:mi><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></m.	2.5	60
13	Multireference perturbation CI I. Extrapolation procedures with CAS or selected zero-order spaces. Theoretical Chemistry Accounts, 1997, 98, 57-63.	1.4	57
14	Rotation and inversion states in thermal E/Z isomerization of aromatic azo compounds. Chemical Physics Letters, 1994, 217, 430-435.	2.6	56
15	Mechanism of thermal Z/E isomerization of substituted N-benzylideneanilines. Nature of the activated complex with an sp-hybridized nitrogen atom. Journal of Organic Chemistry, 1993, 58, 4418-4423.	3.2	54
16	Calibration of the n-electron valence state perturbation theory approach. Journal of Chemical Physics, 2004, 120, 4619-4625.	3.0	49
17	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
18	Theoretical investigations on the solvation process. Theoretica Chimica Acta, 1972, 25, 103-119.	0.8	45

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19	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
20	A convenient decontraction procedure of internally contracted state-specific multireference algorithms. Journal of Chemical Physics, 2006, 124, 234109.	3.0	41
21	Revival of an old structure problem: trithiapentalene - real or time-averaged C2v symmetry?. Journal of the American Chemical Society, 1991, 113, 6449-6451.	13.7	39
22	Multireference perturbation theory can predict a false ground state. Physical Chemistry Chemical Physics, 2010, 12, 5058.	2.8	39
23	The use of local orbitals in multireference calculations. Molecular Physics, 2003, 101, 1389-1398.	1.7	36
24	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
25	An ab initio study of the structure and electronic spectrum of 1,2-dithiete and 1,2-dithiin. Computational and Theoretical Chemistry, 1991, 230, 287-293.	1.5	33
26	Correlation Energy, Thermal Energy, and Entropy Effects in Stabilizing Different Secondary Structures of Peptides. Journal of Physical Chemistry A, 1997, 101, 8571-8574.	2.5	32
27	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
28	Dynamical photoionization observables of the CS molecule: The role of electron correlation. Journal of Chemical Physics, 2014, 140, 204304.	3.0	32
29	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
30	The evaluation of nonadiabatic matrix elements. A comparison of different approximations applied to LiH Xâ€”A 1 Î£ +. Chemical Physics, 1980, 53, 357-363.	1.9	30
31	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
32	The low-lying states of the scandium dimer. Journal of Chemical Physics, 2010, 132, 244306.	3.0	30
33	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
34	Many-body multireference Mï¿½ller?Plesset and Epstein?Nesbet perturbation theory: Fast evaluation of second-order energy contributions. International Journal of Quantum Chemistry, 1996, 60, 167-171.	2.0	28
35	An ab initio multireference perturbation theory study on the manganese dimer. Journal of Chemical Physics, 2008, 128, 244317.	3.0	27
36	Multipole expansions of the electrostatic molecular potential. Theoretica Chimica Acta, 1974, 33, 97-103.	0.8	26

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37	Charge-displacement analysis for excited states. Journal of Chemical Physics, 2014, 140, 054110.	3.0	26
38	Electronic structure investigation of the evanescent AtO⁺ion. Physical Chemistry Chemical Physics, 2014, 16, 9238-9248.	2.8	25
39	Comments on the diabatic representation. Molecular Physics, 1979, 38, 1707-1710.	1.7	24
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.	3.0	24
41	A multireference perturbation theory study on the vertical electronic spectrum of thiophene. Theoretical Chemistry Accounts, 2007, 118, 35-46.	1.4	23
42	A multireference perturbation theory study on the Fe₂molecule: in quest of the ground state. Molecular Physics, 2011, 109, 1503-1509.	1.7	23
43	Multiple complete active space self-consistent field solutions. Molecular Physics, 2003, 101, 1937-1944.	1.7	22
44	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
45	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
46	Diagrammatic formulation of the second-order many-body multipartitioning perturbation theory. International Journal of Quantum Chemistry, 1999, 73, 395-401.	2.0	21
47	Theoretical investigations on the solvation process. Theoretica Chimica Acta, 1973, 29, 93-96.	0.8	20
48	Ab initio study of the photodissociation of nitrosoalkanes and nitrosamines. Journal of the American Chemical Society, 1985, 107, 1617-1622.	13.7	20
49	On the conformation of bipyridine dications and cation radicals. Computational and Theoretical Chemistry, 1986, 139, 213-219.	1.5	20
50	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
51	Photoionization of furan from the ground and excited electronic states. Journal of Chemical Physics, 2016, 144, 084307.	3.0	20
52	Base-induced reactions of isothiazolium salts with active 5-methyl or 5-methylene groups. Journal FÃ¼r Praktische Chemie, Chemiker-Zeitung, 1995, 337, 175-183.	0.5	19
53	Non-orthogonal and orthogonal valence bond wavefunctions in the hydrogen molecule: the diabatic view. Molecular Physics, 2013, 111, 1069-1077.	1.7	19
54	Multireference perturbation CI III. Fast evaluation of the one-particle density matrix. Theoretical Chemistry Accounts, 1998, 100, 324-328.	1.4	18

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55	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
56	Reference conformations for calcium antagonists and agonists of dihydropyridine type. Computational and Theoretical Chemistry, 1990, 205, 1-11.	1.5	16
57	A theoretical description of thetrans-cis conversion in the lowest excited states of diimide. Theoretica Chimica Acta, 1977, 46, 223-235.	0.8	15
58	On the A1Î-X1Î£+ transition in BH: Î›-doubling and vibrational structure Ab initio calculations. Journal of Molecular Spectroscopy, 1981, 87, 303-311.	1.2	15
59	Multireference perturbation CI IV. Selection procedure for one-electron properties. Theoretical Chemistry Accounts, 2001, 105, 259-264.	1.4	15
60	A Simple Approximate Perturbation Approach to Quasi-degenerate Systems. Theoretical Chemistry Accounts, 2006, 116, 434-439.	1.4	14
61	Developments in then-electron valence state perturbation theory. International Journal of Quantum Chemistry, 2006, 106, 686-691.	2.0	13
62	A theoretical study of BeN linear chains: Variational and perturbative approaches. Journal of Chemical Physics, 2009, 131, 034309.	3.0	13
63	Assessment of Multireference Perturbation Methods for Chemical Reaction Barrier Heights. Journal of Physical Chemistry A, 2015, 119, 5490-5495.	2.5	13
64	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
65	The theoretical study of predissociation in diatomics. the case of the O2 B' 3Î£â¯u state. Chemical Physics, 1979, 42, 297-303.	1.9	10
66	Structure and Thermal E-Z Isomerization of Substituted 4-Phenylimino-5-pyrazolones and Hexafluoroacetone Anils.. Bulletin of the Chemical Society of Japan, 1993, 66, 130-134.	3.2	10
67	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
68	Adiabatic and Diabatic Basis Sets in Molecular Calculations. NATO ASI Series Series B: Physics, 1992, , 11-26.	0.2	10
69	On the conformation of the inversion state in the thermal E,Z isomerization of aromatic azomethines. Journal of the Chemical Society Chemical Communications, 1991, , 295.	2.0	9
70	Geometry optimization within a localized CAS-SCF approach. Chemical Physics Letters, 2003, 371, 49-55.	2.6	9
71	On the direct calculation of the time evolution of excited molecular states in the presence of nonadiabatic interactions. Chemical Physics, 1978, 34, 103-112.	1.9	8
72	Local orbitals for quasi-degenerate systems. Computational and Theoretical Chemistry, 2004, 709, 1-10.	1.5	8

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73	Alternative paths in the ring opening of oxadiaziridine: The diimide N-oxide versus the oxodiimide rearrangement. Theoretica Chimica Acta, 1978, 49, 13-23.	0.8	7
74	Changes in electronically excited states and photochemistry of troponoids on complexation with acids. Journal of Photochemistry and Photobiology A: Chemistry, 1991, 61, 329-342.	3.9	7
75	Azoxy compounds and oxadiaziridines. An ab initio study of the ring closure reactions and the cis-trans isomerizations. The Journal of Physical Chemistry, 1977, 81, 1876-1882.	2.9	6
76	The cisâ€"trans thermal and photochemical interconversion mechanism in the dimide N-oxide. A comparison of the results obtainable with different ab initio calculation techniques. Chemical Physics, 1977, 24, 251-261.	1.9	5
77	Torsional barriers and the electronic spectrum of nitrosomethane. Chemical Physics Letters, 1979, 63, 352-354.	2.6	5
78	Contracted and supercontracted basis sets in the theoretical treatment of coordination compounds: The cyclopentadienyl anion and ferrocene. Chemical Physics Letters, 1988, 153, 507-510.	2.6	5
79	Zur Konformation von Calciumantagonisten und â€agonisten vom Dihydropyridintyp. Zeitschrift FÃ¼r Chemie, 1988, 28, 326-327.	0.0	5
80	Simplified treatment of organic substituents in SCFâ€CI calculations. The methyl group. Journal of Chemical Physics, 1987, 87, 1653-1660.	3.0	4
81	Reply to the â€˜Comment on â€œMulticonfigurational perturbation theory can predict a false ground stateâ€â€™ by J. Soto, F. Avila, J. C. Otero and J. F. Arenas, Phys. Chem. Chem. Phys., 2011, DOI: 10.1039/C0CP01917H. Physical Chemistry Chemical Physics, 2011, 13, 7232.	2.8	4
82	A priori complete active space self consistent field localized orbitals: an application on linear polyenes. Molecular Physics, 2006, 104, 691-700.	1.7	3
83	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
84	On the conformational structure of amrinone and milrinone. European Journal of Medicinal Chemistry, 1987, 22, 569-572.	5.5	1