Renzo Cimiraglia

List of Publications by Year
in descending order

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	Photoionization of furan from the ground and excited electronic states. Journal of Chemical Physics, 2016, 144, 084307.	3.0	20
2	Assessment of Multireference Perturbation Methods for Chemical Reaction Barrier Heights. Journal of Physical Chemistry A, 2015, 119, 5490-5495.	2.5	13
3	Charge-displacement analysis for excited states. Journal of Chemical Physics, 2014, 140, 054110.	3.0	26
4	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
5	Dynamical photoionization observables of the CS molecule: The role of electron correlation. Journal of Chemical Physics, 2014, 140, 204304.	3.0	32
6	The Dalton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	14.6	1,166
7	Electronic structure investigation of the evanescent AtO^{+} ion. Physical Chemistry Chemical Physics, 2014, 16, 9238-9248.	2.8	25
8	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
9	Non-orthogonal and orthogonal valence bond wavefunctions in the hydrogen molecule: the diabatic view. Molecular Physics, 2013, 111, 1069-1077.	1.7	19
10	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
11	A multireference perturbation theory study on the Fe_2 molecule: in quest of the ground state. Molecular Physics, 2011, 109, 1503-1509.	1.7	23
12	Reply to the 'Comment on "Multiconfigurational perturbation theory can predict a false ground state"' 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
13	The low-lying states of the scandium dimer. Journal of Chemical Physics, 2010, 132, 244306.	3.0	30
14	Merging multireference perturbation and density-functional theories by means of range separation: Potential curves for Be_2, Mg_2.	2.5	60
15	Multireference perturbation theory can predict a false ground state. Physical Chemistry Chemical Physics, 2010, 12, 5058.	2.8	39
16	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
17	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.	1.5	10
18	A theoretical study of BeN linear chains: Variational and perturbative approaches. Journal of Chemical Physics, 2009, 131, 034309.	3.0	13

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19	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.	3.3	84
20	An ab initio multireference perturbation theory study on the manganese dimer. Journal of Chemical Physics, 2008, 128, 244317.	3.0	27
21	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
22	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
23	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
24	New perspectives in multireference perturbation theory: the n-electron valence state approach. Theoretical Chemistry Accounts, 2007, 117, 743-754.	1.4	238
25	A multireference perturbation theory study on the vertical electronic spectrum of thiophene. Theoretical Chemistry Accounts, 2007, 118, 35-46.	1.4	23
26	Developments in then-electron valence state perturbation theory. International Journal of Quantum Chemistry, 2006, 106, 686-691.	2.0	13
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	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
29	A Simple Approximate Perturbation Approach to Quasi-degenerate Systems. Theoretical Chemistry Accounts, 2006, 116, 434-439.	1.4	14
30	Third-order multireference perturbation theory: The n-electron valence state perturbation-theory approach. Journal of Chemical Physics, 2006, 124, 054108.	3.0	151
31	A convenient decontraction procedure of internally contracted state-specific multireference algorithms. Journal of Chemical Physics, 2006, 124, 234109.	3.0	41
32	A priori complete active space self consistent field localized orbitals: an application on linear polyenes. Molecular Physics, 2006, 104, 691-700.	1.7	3
33	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
34	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
35	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
36	Local orbitals for quasi-degenerate systems. Computational and Theoretical Chemistry, 2004, 709, 1-10.	1.5	8

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37	Calibration of the n-electron valence state perturbation theory approach. Journal of Chemical Physics, 2004, 120, 4619-4625.	3.0	49
38	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
39	Geometry optimization within a localized CAS-SCF approach. Chemical Physics Letters, 2003, 371, 49-55.	2.6	9
40	The use of local orbitals in multireference calculations. Molecular Physics, 2003, 101, 1389-1398.	1.7	36
41	Multiple complete active space self-consistent field solutions. Molecular Physics, 2003, 101, 1937-1944.	1.7	22
42	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
43	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.	3.0	61
44	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
45	Multireference perturbation CI IV. Selection procedure for one-electron properties. Theoretical Chemistry Accounts, 2001, 105, 259-264.	1.4	15
46	N-electron valence state perturbation theory: a fast implementation of the strongly contracted variant. Chemical Physics Letters, 2001, 350, 297-305.	2.6	689
47	On a mixed Mï¿½ller–Plesset Epstein–Nesbet partition of the Hamiltonian to be used in multireference perturbation configuration interaction. Chemical Physics Letters, 2000, 317, 472-480.	2.6	41
48	Diagrammatic formulation of the second-order many-body multipartitioning perturbation theory. International Journal of Quantum Chemistry, 1999, 73, 395-401.	2.0	21
49	Multireference perturbation CI III. Fast evaluation of the one-particle density matrix. Theoretical Chemistry Accounts, 1998, 100, 324-328.	1.4	18
50	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
51	Multireference perturbation CI I. Extrapolation procedures with CAS or selected zero-order spaces. Theoretical Chemistry Accounts, 1997, 98, 57-63.	1.4	57
52	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
53	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
54	Base-induced reactions of isothiazolium salts with active 5-methyl or 5-methylene groups. Journal Für Praktische Chemie, Chemiker-Zeitung, 1995, 337, 175-183.	0.5	19

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55	Rotation and inversion states in thermal E/Z isomerization of aromatic azo compounds. Chemical Physics Letters, 1994, 217, 430-435.	2.6	56
56	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
57	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
58	Adiabatic and Diabatic Basis Sets in Molecular Calculations. NATO ASI Series Series B: Physics, 1992, , 11-26.	0.2	10
59	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
60	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
61	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
62	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
63	Reference conformations for calcium antagonists and agonists of dihydropyridine type. Computational and Theoretical Chemistry, 1990, 205, 1-11.	1.5	16
64	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
65	Zur Konformation von Calciumantagonisten und €agonisten vom Dihydropyridintyp. Zeitschrift für Chemie, 1988, 28, 326-327.	0.0	5
66	Simplified treatment of organic substituents in SCF€CI calculations. The methyl group. Journal of Chemical Physics, 1987, 87, 1653-1660.	3.0	4
67	Recent advances in multireference second order perturbation CI: The CIPSI method revisited. Journal of Computational Chemistry, 1987, 8, 39-47.	3.3	117
68	On the conformational structure of amrinone and milrinone. European Journal of Medicinal Chemistry, 1987, 22, 569-572.	5.5	1
69	On the conformation of bipyridine dications and cation radicals. Computational and Theoretical Chemistry, 1986, 139, 213-219.	1.5	20
70	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
71	Ab initio study of the photodissociation of nitrosoalkanes and nitrosamines. Journal of the American Chemical Society, 1985, 107, 1617-1622.	13.7	20
72	On the $A^1\Pi$-$X^1\Sigma^+$ transition in BH: Λ-doubling and vibrational structure Ab initio calculations. Journal of Molecular Spectroscopy, 1981, 87, 303-311.	1.2	15

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73	The evaluation of nonadiabatic matrix elements. A comparison of different approximations applied to LiH X—A 1 Σ +. Chemical Physics, 1980, 53, 357-363.	1.9	30
74	Comments on the diabatic representation. Molecular Physics, 1979, 38, 1707-1710.	1.7	24
75	Torsional barriers and the electronic spectrum of nitrosomethane. Chemical Physics Letters, 1979, 63, 352-354.	2.6	5
76	The theoretical study of predissociation in diatomics. the case of the O2 B' 3Σ—u state. Chemical Physics, 1979, 42, 297-303.	1.9	10
77	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
78	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
79	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
80	The cis—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
81	A theoretical description of thetrans-cis conversion in the lowest excited states of diimide. Theoretica Chimica Acta, 1977, 46, 223-235.	0.8	15
82	Multipole expansions of the electrostatic molecular potential. Theoretica Chimica Acta, 1974, 33, 97-103.	0.8	26
83	Theoretical investigations on the solvation process. Theoretica Chimica Acta, 1973, 29, 93-96.	0.8	20
84	Theoretical investigations on the solvation process. Theoretica Chimica Acta, 1972, 25, 103-119.	0.8	45