Rajat K Chaudhuri

List of Publications by Year
in descending order

84	1,543	304602 22	377752 34
papers	citations	h-index	g-index

85	85	85	837
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The improved virtual orbital-complete active space configuration interaction method, a â€œpackageableâ€• efficientab initiomany-body method for describing electronically excited states. Journal of Chemical Physics, 2001, 114, 2592-2600.	1.2	95
2	Applications of multireference perturbation theory to potential energy surfaces by optimal partitioning ofH: Intruder states avoidance and convergence enhancement. Journal of Chemical Physics, 1995, 103, 4990-5010.	1.2	93
3	Hybrid approach to relativistic Gaussian basis functions: Theory and applications. Physical Review A, 1999, 59, 1187-1196.	1.0	67
4	Comparison of low-order multireference many-body perturbation theories. Journal of Chemical Physics, 2005, 122, 134105.	1.2	62
5	Convergence behavior of multireference perturbation theory: Forced degeneracy and optimization partitioning applied to the beryllium atom. Physical Review A, 1996, 54, 343-356.	1.0	55
6	Molecular applications of state-specific multireference perturbation theory to HF, H2O, H2S, C2, and N2 molecules. Journal of Chemical Physics, 2008, 129, 024108.	1.2	50
7	Global threeâ€dimensional potential energy surfaces of H2S from the ab initio effective valence shell Hamiltonian method. Journal of Chemical Physics, 1996, 105, 8754-8768.	1.2	46
8	Potential energy curve for isomerization of N2H2 and C2H4 using the improved virtual orbital multireference MÃ¸llerâ€“Plesset perturbation theory. Journal of Chemical Physics, 2008, 128, 144304.	1.2	44
9	Comparison of the perturbative convergence with multireference MÃ¶llerâ€“Plesset, Epsteinâ€“Nesbet, forced degenerate and optimized zeroth order partitionings: The excited BeH2surface. Journal of Chemical Physics, 1997, 106, 4067-4081.	1.2	43
10	Application of state-specific multireference MÃ¸llerâ€“Plesset perturbation theory to nonsinglet states. Journal of Chemical Physics, 2009, 130, 014101.	1.2	37
11	Application of the effective valence shell Hamiltonian method to accurate estimation of valence and Rydberg states oscillator strengths and excitation energies for Ï€ electron systems. Journal of Chemical Physics, 1997, 106, 9252-9264.	1.2	33
12	Stateâ€specific multireference perturbation theory with improved virtual orbitals: Taming the ground state of <scp>F</scp>₂, <scp>B</scp>e_{2,} and <scp>N</scp>₂. Journal of Computational Chemistry, 2015, 36, 907-925.	1.5	33
13	Electric Quadrupole Moments of theDStates of Alkaline-Earth-Metal Ions. Physical Review Letters, 2006, 96, 193001.	2.9	31
14	Geometry Optimization of Radicaloid Systems Using Improved Virtual Orbital-Complete Active Space Configuration Interaction (IVO-CASCI) Analytical Gradient Method. Journal of Physical Chemistry A, 2011, 115, 3665-3678.	1.1	31
15	Stateâ€specific multireference perturbation theory: development and present status. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 266-291.	6.2	31
16	Application of relativistic Fock-space coupled-cluster theory to study Li and Li-like ions in plasma. Physical Review A, 2012, 85, .	1.0	30
17	Application of improved virtual orbital based multireference methods to N2, LiF, and C4H6 systems. Journal of Chemical Physics, 2008, 129, 244108.	1.2	29
18	Electronic structure of the calcium monohydroxide radical. Journal of Chemical Physics, 2005, 122, 044317.	1.2	28

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19	Comparison of high order perturbative convergence of multireference perturbation methods: Application to singlet states of CH2. Journal of Chemical Physics, 1997, 107, 6699-6711.	1.2	27
20	On the extensivity of the roots of effective Hamiltonians in many-body formalisms employing incomplete model spaces. Chemical Physics Letters, 1989, 163, 165-170.	1.2	25
21	A comparative study of core-extensive and coreâ€"valence-extensive coupled-cluster theories for energy differences: Excitation energies. Chemical Physics Letters, 1990, 173, 181-186.	1.2	23
22	Reappraisal ofciseffect in 1,2-dihaloethenes: An improved virtual orbital multireference approach. Journal of Chemical Physics, 2008, 129, 064101.	1.2	23
23	Relativistic coupled cluster calculations of the energies for rubidium and cesium atoms. Journal of Chemical Physics, 2003, 119, 10633-10637.	1.2	20
24	Relativistic effective valence shell Hamiltonian method: Excitation and ionization energies of heavy metal atoms. Journal of Chemical Physics, 2005, 122, 204111.	1.2	20
25	Relativistic coupled cluster method. European Physical Journal D, 2006, 37, 171-176.	0.6	20
26	Theoretical Studies of the Ground and Excited State Structures of Stilbene. Journal of Physical Chemistry A, 2013, 117, 9424-9434.	1.1	19
27	Ionization potentials of beryllium-like ions from the relativistic coupled-cluster-based linear response theory. Journal of Physics B: Atomic, Molecular and Optical Physics, 2000, 33, 5129-5138.	0.6	18
28	Study of the Ground State Dissociation of Diatomic Molecular Systems Using State-Specific Multireference Perturbation Theory: A Brillouinâ˜'Wigner Scheme. Journal of Chemical Theory and Computation, 2010, 6, 662-682.	2.3	18
29	Prediction of electronic structure of organic radicaloid anions using efficient, economical multireference gradient approach. Physical Chemistry Chemical Physics, 2011, 13, 7514.	1.3	18
30	A critical comparison of theoretical and experimental electronic spectrum and potential energy curves of HF molecule and its positive and negative ions. Computational and Theoretical Chemistry, 2001, 547, 83-96.	1.5	16
31	Ab Initio Multireference Investigation of Disjoint Diradicals: Singlet versus Triplet Ground States. ChemPhysChem, 2011, 12, 2791-2797.	1.0	16
32	Application of an efficient multireference approach to free-base porphin and metalloporphyrins: Ground, excited, and positive ion states. Journal of Chemical Physics, 2011, 135, 084118.	1.2	16
33	Spectral lines behavior of Be I and Na I isoelectronic sequence in Debye plasma environment. Physics of Plasmas, 2012, 19, .	0.7	16
34	Revisiting the â€˜cis-effectâ€™ in 1,2-difluoro derivatives of ethylene and diazene usingab initiomultireference methods. Molecular Physics, 2014, 112, 3206-3224.	0.8	16
35	Taming the Electronic Structure of Diradicals through the Window of Computationally Cost Effective Multireference Perturbation Theory. Journal of Physical Chemistry A, 2016, 120, 5897-5916.	1.1	16
36	A new nonperturbative theory of core-hole ionizations: a compact cluster-expansion technique for treating relaxation effects. Chemical Physics Letters, 1990, 172, 515-521.	1.2	15

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37	Relativistic coupled-cluster-based linear response theory for ionization potentials of alkali-metal and alkaline-earth-metal atoms. Physical Review A, 1999, 60, 246-252.	1.0	15
38	Determination of conformational energy differences of propynlidyne isomers using the effective valence shell Hamiltonian method. Journal of Chemical Physics, 2000, 112, 9301-9309.	1.2	15
39	Geometry optimization using improved virtual orbitals: A complete active space numerical gradient approach. Journal of Chemical Physics, 2007, 126, 114103.	1.2	14
40	Re-appraisal of the P,T-odd interaction constant W d in YbF: Relativistic configuration interaction approach. Pramana - Journal of Physics, 2009, 73, 581-586.	0.9	14
41	Application of relativistic coupled cluster linear response theory to helium-like ions embedded in plasma environment. Journal of Physics B: Atomic, Molecular and Optical Physics, 2011, 44, 165701.	0.6	14
42	Improved virtual orbitals in state specific multireference perturbation theory for prototypes of quasidegenerate electronic structure. Journal of Chemical Physics, 2017, 146, 064111.	1.2	14
43	RELATIVISTIC AND CORRELATION EFFECTS IN ATOMS. Journal of Theoretical and Computational Chemistry, 2005, 04, 1-20.	1.8	13
44	Investigation of Low-Lying States of Oxygen Molecule via Second-Order Multireference Perturbation Theory: A State-Specific Approach. Journal of Physical Chemistry A, 2009, 113, 5972-5984.	1.1	13
45	Secondâ€order stateâ€specific multireference MÃ¸ller Plesset perturbation theory: Application to energy surfaces of diimide, ethylene, butadiene, and cyclobutadiene. Journal of Computational Chemistry, 2011, 32, 325-337.	1.5	13
46	Relativistic state-specific multireference coupled cluster theory description for bond-breaking energy surfaces. Journal of Chemical Physics, 2016, 145, 124303.	1.2	13
47	Ab initio calculations of forbidden transition amplitudes and lifetimes of the low-lying states in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msup><mml:mi mathvariant="normal">V</mml:mi><mml:mrow><mml:mn>4</mml:mn><mml:mo>+</mml:mo></mml:mrow></mml:msup></mml:mrow	1.0	12
48	Molecular applications of analytical gradient approach for the improved virtual orbital-complete active space configuration interaction method. Journal of Chemical Physics, 2010, 132, 034105.	1.2	12
49	A critical analysis of the ground and excited electronic states of transition metal nitrides using the relativistic effective Hamiltonian method. Journal of Chemical Physics, 2003, 119, 5995-6002.	1.2	11
50	Generation of potential energy curves for the XÎ£g+1, BÎ”g+1, and Bâ€²Î£g+1 states of C2 using the effective valence shell Hamiltonian method. Journal of Chemical Physics, 2005, 122, 154310.	1.2	11
51	Second-Order State-Specific Multireference MÃ¸llerâ^'Plesset Perturbation Theory (SS-MRMPPT) Applied to Geometry Optimization. Journal of Physical Chemistry A, 2010, 114, 3668-3682.	1.1	11
52	Description of C₂ dissociation using a naive treatment of dynamical correlation in the presence of quasidegeneracy of varying degree. Molecular Physics, 2017, 115, 2789-2806.	0.8	11
53	Improved virtual orbital multireference MÃ¸llerâ€“Plesset study of the ground and excited electronic states of protonated acetylene, C2H3+. Journal of Chemical Physics, 2008, 129, 054308.	1.2	10
54	Studies on m-benzyne and phenol via improved virtual orbital-complete active space configuration interaction (IVO-CASCI) analytical gradient method. Chemical Physics Letters, 2010, 491, 102-108.	1.2	10

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55	Dissociation of homonuclear diatomic halogens via multireference coupled cluster calculations. Molecular Physics, 2014, 112, 2720-2736.	0.8	10
56	Comparative studies using coupled-cluster and unitary coupled-cluster methods: nuclear quadrupole moment, hyperfine constants and transition properties of27Al. Journal of Physics B: Atomic, Molecular and Optical Physics, 2005, 38, 4185-4194.	0.6	9
57	Relativistic state-specific multireference perturbation theory incorporating improved virtual orbitals: Application to the ground state single-bond dissociation. Journal of Computational Chemistry, 2015, 36, 1954-1972.	1.5	9
58	Application of the effective valence shell Hamiltonian method to accurate estimation of oscillator strengths and excitation energies of Mg-like ions. Journal of Chemical Physics, 1998, 108, 2556-2562.	1.2	8
59	Reappraisal of Nuclear Quadrupole Moments of Atomic Halogens via Relativistic Coupled Cluster Linear Response Theory for the Ionization Process. Journal of Physical Chemistry A, 2013, 117, 12616-12627.	1.1	8
60	Evaluation of analytic molecular orbital derivatives and gradients using the effective valence shell Hamiltonian method. Journal of Chemical Physics, 1998, 109, 9685-9693.	1.2	7
61	Theoretical Study on the Electronic States of Formylcarbene (HCÂ·CHO) and Triplet Ketene (H₂ CCO) and the Ultraviolet Absorption Spectra Attributable to These Molecules. Journal of Physical Chemistry A, 2008, 112, 4399-4404.	1.1	7
62	State-specific complete active space multireference MÃ¸llerâ€“Plesset perturbation approach for multireference situations: illustrating the bond breaking in hydrogen halides. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	7
63	Multireference perturbation theory with improved virtual orbitals for radicals: More degeneracies, more problems. International Journal of Quantum Chemistry, 2019, 119, e25776.	1.0	7
64	Taming the excited states of butadiene, hexatriene, and octatetraene using state specific multireference perturbation theory with density functional theory orbitals. Journal of Chemical Physics, 2020, 152, 244105.	1.2	7
65	Valence universal multireference coupled cluster calculations of the properties of indium in its ground and excited states. Journal of Physics B: Atomic, Molecular and Optical Physics, 2011, 44, 065003.	0.6	6
66	State specific multireference MÃ¸llerâ€“Plesset perturbation theory: A few applications to ground, excited and ionized states. Chemical Physics, 2012, 401, 15-26.	0.9	6
67	A simplified ab initio treatment of diradicaloid structures produced from stretching and breaking chemical bonds. Physical Chemistry Chemical Physics, 2017, 19, 22282-22301.	1.3	6
68	The Excited and Ion States of Allene. ACS Symposium Series, 2002, , 154-175.	0.5	5
69	Study of equilibrium geometries of diradicaloid systems via state specific multireference MÃ¸llerâ€“Plesset perturbation theory (SS-MRMPPT). Chemical Physics Letters, 2010, 488, 229-234.	1.2	5
70	A simplified account of the correlation effects to bond breaking processes: The Brillouin-Wigner perturbation theory using a multireference formulation. Journal of Chemical Physics, 2019, 151, 064114.	1.2	5
71	Theoretical Study on the Ground and Excited States of Dicyanocarbene (C3N2) and Its Isomers:â€‰ A Low-Temperature Matrix Emission Spectrum Attributable to 3-Cyano-2H-azirenylidene. Journal of Physical Chemistry A, 2007, 111, 4849-4854.	1.1	4
72	Four-Component Relativistic State-Specific Multireference Perturbation Theory with a Simplified Treatment of Static Correlation. Journal of Physical Chemistry A, 2017, 121, 1487-1501.	1.1	4

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73	Coupled Cluster Calculations of the Ground and Excited Electronic States Using Two- and Four-Component Relativistic Spinors. International Journal of Molecular Sciences, 2003, 4, 586-594.	1.8	3
74	Combined complete active space configuration interaction and perturbation theory applied to conformational energy prototypes: Rotation and inversion barriers. Computational and Theoretical Chemistry, 2017, 1120, 56-78.	1.1	3
75	Taming the Electronic Structure of Lead and Eka-lead (Flerovium) by the Relativistic Coupled Cluster Method. Journal of Physical Chemistry A, 2013, 117, 8555-8567.	1.1	2
76	Communication: Viewing the ground and excited electronic structures of platinum and its ion through the window of relativistic coupled cluster method. Journal of Chemical Physics, 2017, 146, 011102.	1.2	2
77	Equation of motion approach for describing allowed transitions in Ne and Al3+ under classical and quantum plasmas. Physics of Plasmas, 2018, 25, .	0.7	2
78	RANDOM PHASE APPROXIMATION FOR ALLOWED AND PARITY NON-CONSERVING ELECTRIC DIPOLE TRANSITION AMPLITUDES AND ITS CONNECTION WITH MANY-BODY PERTURBATION THEORY AND COUPLED-CLUSTER THEORY. Journal of Theoretical and Computational Chemistry, 2006, 05, 945-956.	1.8	1
79	Effects of partial triple excitations in atomic coupled cluster calculations. Chemical Physics Letters, 2007, 442, 150-156.	1.2	1
80	Profiling the binding motif between Be and Mg in the ground state via a single-reference coupled cluster method. Molecular Physics, 2015, 113, 1387-1395.	0.8	1
81	Fock-space multireference coupled cluster calculations of Auger energies of noble gas elements using relativistic spinors. Journal of Chemical Physics, 2019, 151, 074114.	1.2	1
82	A Fock space coupled cluster based probing of the single- and double-ionization profiles for the poly-cyclic aromatic hydrocarbons and conjugated polyenes. Journal of Chemical Physics, 2021, 154, 114106.	1.2	1
83	Optical frequency standard with Sr⁺: A theoretical many-body approach. , 2006, , .		0
84	Description of the Methylene Amidogene Radical and Its Anion with an Economical Treatment of Correlation Effects Using Density Functional Theory Orbitals. Journal of Physical Chemistry A, 2021, 125, 543-558.	1.1	0