

# Rajat K Chaudhuri

## List of Publications by Year in descending order

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84  
papers

1,543  
citations

304602

22  
h-index

377752

34  
g-index

85  
all docs

85  
docs citations

85  
times ranked

837  
citing authors

#	ARTICLE	IF	CITATIONS
1	Description of the Methylene Amidogene Radical and Its Anion with an Economical Treatment of Correlation Effects Using Density Functional Theory Orbitals. <i>Journal of Physical Chemistry A</i> , 2021, 125, 543-558.	1.1	0
2	A Fock space coupled cluster based probing of the single- and double-ionization profiles for the poly-cyclic aromatic hydrocarbons and conjugated polyenes. <i>Journal of Chemical Physics</i> , 2021, 154, 114106.	1.2	1
3	Taming the excited states of butadiene, hexatriene, and octatetraene using state specific multireference perturbation theory with density functional theory orbitals. <i>Journal of Chemical Physics</i> , 2020, 152, 244105.	1.2	7
4	A simplified account of the correlation effects to bond breaking processes: The Brillouin-Wigner perturbation theory using a multireference formulation. <i>Journal of Chemical Physics</i> , 2019, 151, 064114.	1.2	5
5	Fock-space multireference coupled cluster calculations of Auger energies of noble gas elements using relativistic spinors. <i>Journal of Chemical Physics</i> , 2019, 151, 074114.	1.2	1
6	Multireference perturbation theory with improved virtual orbitals for radicals: More degeneracies, more problems. <i>International Journal of Quantum Chemistry</i> , 2019, 119, e25776.	1.0	7
7	Equation of motion approach for describing allowed transitions in Ne and Al <sup>3+</sup> under classical and quantum plasmas. <i>Physics of Plasmas</i> , 2018, 25, .	0.7	2
8	Four-Component Relativistic State-Specific Multireference Perturbation Theory with a Simplified Treatment of Static Correlation. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1487-1501.	1.1	4
9	Improved virtual orbitals in state specific multireference perturbation theory for prototypes of quasidegenerate electronic structure. <i>Journal of Chemical Physics</i> , 2017, 146, 064111.	1.2	14
10	Description of C <sub>2</sub> dissociation using a naive treatment of dynamical correlation in the presence of quasidegeneracy of varying degree. <i>Molecular Physics</i> , 2017, 115, 2789-2806.	0.8	11
11	Combined complete active space configuration interaction and perturbation theory applied to conformational energy prototypes: Rotation and inversion barriers. <i>Computational and Theoretical Chemistry</i> , 2017, 1120, 56-78.	1.1	3
12	Communication: Viewing the ground and excited electronic structures of platinum and its ion through the window of relativistic coupled cluster method. <i>Journal of Chemical Physics</i> , 2017, 146, 011102.	1.2	2
13	A simplified ab initio treatment of diradicaloid structures produced from stretching and breaking chemical bonds. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 22282-22301.	1.3	6
14	Relativistic state-specific multireference coupled cluster theory description for bond-breaking energy surfaces. <i>Journal of Chemical Physics</i> , 2016, 145, 124303.	1.2	13
15	State-specific multireference perturbation theory: development and present status. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2016, 6, 266-291.	6.2	31
16	Taming the Electronic Structure of Diradicals through the Window of Computationally Cost Effective Multireference Perturbation Theory. <i>Journal of Physical Chemistry A</i> , 2016, 120, 5897-5916.	1.1	16
17	Relativistic state-specific multireference perturbation theory incorporating improved virtual orbitals: Application to the ground state single-bond dissociation. <i>Journal of Computational Chemistry</i> , 2015, 36, 1954-1972.	1.5	9
18	Profiling the binding motif between Be and Mg in the ground state via a single-reference coupled cluster method. <i>Molecular Physics</i> , 2015, 113, 1387-1395.	0.8	1

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19	State-specific multireference perturbation theory with improved virtual orbitals: Taming the ground state of $F_2$ , $B_2$ and $N_2$ . Journal of Computational Chemistry, 2015, 36, 907-925.	1.5	33
20	Revisiting the $\tilde{c}_{cis}$ effect™ in 1,2-difluoro derivatives of ethylene and diazene using <i>ab initio</i> multireference methods. Molecular Physics, 2014, 112, 3206-3224.	0.8	16
21	Dissociation of homonuclear diatomic halogens via multireference coupled cluster calculations. Molecular Physics, 2014, 112, 2720-2736.	0.8	10
22	Theoretical Studies of the Ground and Excited State Structures of Stilbene. Journal of Physical Chemistry A, 2013, 117, 9424-9434.	1.1	19
23	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
24	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
25	Spectral lines behavior of Be I and Na I isoelectronic sequence in Debye plasma environment. Physics of Plasmas, 2012, 19, .	0.7	16
26	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
27	State-specific complete active space multireference Møller-Plesset perturbation approach for multireference situations: illustrating the bond breaking in hydrogen halides. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	7
28	State specific multireference Møller-Plesset perturbation theory: A few applications to ground, excited and ionized states. Chemical Physics, 2012, 401, 15-26.	0.9	6
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	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
31	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
32	Ab Initio Multireference Investigation of Disjoint Diradicals: Singlet versus Triplet Ground States. ChemPhysChem, 2011, 12, 2791-2797.	1.0	16
33	Second-order state-specific multireference Møller Plesset perturbation theory: Application to energy surfaces of diimide, ethylene, butadiene, and cyclobutadiene. Journal of Computational Chemistry, 2011, 32, 325-337.	1.5	13
34	Application of an efficient multireference approach to free-base porphyrin and metalloporphyrins: Ground, excited, and positive ion states. Journal of Chemical Physics, 2011, 135, 084118.	1.2	16
35	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
36	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	Optical frequency standard with $\text{Sr}^{+}$ : A theoretical many-body approach. , 2006, , .		0
56	Electric Quadrupole Moments of the D States of Alkaline-Earth-Metal Ions. Physical Review Letters, 2006, 96, 193001.	2.9	31
57	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
58	Electronic structure of the calcium monohydroxide radical. Journal of Chemical Physics, 2005, 122, 044317.	1.2	28
59	Comparison of low-order multireference many-body perturbation theories. Journal of Chemical Physics, 2005, 122, 134105.	1.2	62
60	Relativistic effective valence shell Hamiltonian method: Excitation and ionization energies of heavy metal atoms. Journal of Chemical Physics, 2005, 122, 204111.	1.2	20
61	RELATIVISTIC AND CORRELATION EFFECTS IN ATOMS. Journal of Theoretical and Computational Chemistry, 2005, 04, 1-20.	1.8	13
62	Generation of potential energy curves for the $X^1\Sigma^+g+1$ , $B^1\Pi^+g+1$ , and $B^2\Sigma^+g+1$ states of $C_2$ using the effective valence shell Hamiltonian method. Journal of Chemical Physics, 2005, 122, 154310.	1.2	11
63	Comparative studies using coupled-cluster and unitary coupled-cluster methods: nuclear quadrupole moment, hyperfine constants and transition properties of $^{27}Al$ . Journal of Physics B: Atomic, Molecular and Optical Physics, 2005, 38, 4185-4194.	0.6	9
64	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
65	Relativistic coupled cluster calculations of the energies for rubidium and cesium atoms. Journal of Chemical Physics, 2003, 119, 10633-10637.	1.2	20
66	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
67	The Excited and Ion States of Allene. ACS Symposium Series, 2002, , 154-175.	0.5	5
68	The improved virtual orbital-complete active space configuration interaction method, a $\epsilon$ -packageable efficient many-body method for describing electronically excited states. Journal of Chemical Physics, 2001, 114, 2592-2600.	1.2	95
69	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
70	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
71	Determination of conformational energy differences of propynylidyne isomers using the effective valence shell Hamiltonian method. Journal of Chemical Physics, 2000, 112, 9301-9309.	1.2	15
72	Hybrid approach to relativistic Gaussian basis functions: Theory and applications. Physical Review A, 1999, 59, 1187-1196.	1.0	67

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73	Relativistic coupled-cluster-based linear response theory for ionization potentials of alkali-metal and alkaline-earth-metal atoms. <i>Physical Review A</i> , 1999, 60, 246-252.	1.0	15
74	Evaluation of analytic molecular orbital derivatives and gradients using the effective valence shell Hamiltonian method. <i>Journal of Chemical Physics</i> , 1998, 109, 9685-9693.	1.2	7
75	Application of the effective valence shell Hamiltonian method to accurate estimation of oscillator strengths and excitation energies of Mg-like ions. <i>Journal of Chemical Physics</i> , 1998, 108, 2556-2562.	1.2	8
76	Application of the effective valence shell Hamiltonian method to accurate estimation of valence and Rydberg states oscillator strengths and excitation energies for $\tilde{\epsilon}$ electron systems. <i>Journal of Chemical Physics</i> , 1997, 106, 9252-9264.	1.2	33
77	Comparison of high order perturbative convergence of multireference perturbation methods: Application to singlet states of CH <sub>2</sub> . <i>Journal of Chemical Physics</i> , 1997, 107, 6699-6711.	1.2	27
78	Comparison of the perturbative convergence with multireference Møller-Plesset, Epstein-Nesbet, forced degenerate and optimized zeroth order partitionings: The excited BeH <sub>2</sub> surface. <i>Journal of Chemical Physics</i> , 1997, 106, 4067-4081.	1.2	43
79	Convergence behavior of multireference perturbation theory: Forced degeneracy and optimization partitioning applied to the beryllium atom. <i>Physical Review A</i> , 1996, 54, 343-356.	1.0	55
80	Global three-dimensional potential energy surfaces of H <sub>2</sub> S from the ab initio effective valence shell Hamiltonian method. <i>Journal of Chemical Physics</i> , 1996, 105, 8754-8768.	1.2	46
81	Applications of multireference perturbation theory to potential energy surfaces by optimal partitioning of H: Intruder states avoidance and convergence enhancement. <i>Journal of Chemical Physics</i> , 1995, 103, 4990-5010.	1.2	93
82	A comparative study of core-extensive and core-valence-extensive coupled-cluster theories for energy differences: Excitation energies. <i>Chemical Physics Letters</i> , 1990, 173, 181-186.	1.2	23
83	A new nonperturbative theory of core-hole ionizations: a compact cluster-expansion technique for treating relaxation effects. <i>Chemical Physics Letters</i> , 1990, 172, 515-521.	1.2	15
84	On the extensivity of the roots of effective Hamiltonians in many-body formalisms employing incomplete model spaces. <i>Chemical Physics Letters</i> , 1989, 163, 165-170.	1.2	25