Debashis Mukherjee

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/7633071/publications.pdf

Version: 2024-02-01

75	5,256	117625	85541
papers	citations	34 h-index	71 g-index

75	75	75	1006
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	On the connectivity criteria in the open-shell coupled-cluster theory for general model spaces. Physics Reports, 1987, 151, 93-127.	25.6	453
2	A size-consistent state-specific multireference coupled cluster theory: Formal developments and molecular applications. Journal of Chemical Physics, 1999, 110, 6171-6188.	3.0	393
3	Use of Cluster Expansion Methods in the Open-Shell Correlation Problem. Advances in Quantum Chemistry, 1989, 20, 291-373.	0.8	353
4	Application of cluster expansion techniques to open shells: Calculation of difference energies. Journal of Chemical Physics, 1984, 80, 5058-5069.	3.0	283
5	Correlation problem in open-shell atoms and molecules. Molecular Physics, 1975, 30, 1861-1888.	1.7	282
6	Applications of a non-perturbative many-body formalism to general open-shell atomic and molecular problems: calculation of the ground and the lowest Ï€-Ï€* singlet and triplet energies and the first ionization potential of trans-butadiene. Molecular Physics, 1977, 33, 955-969.	1.7	281
7	Cumulant expansion of the reduced density matrices. Journal of Chemical Physics, 1999, 110, 2800-2809.	3.0	241
8	Normal order and extended Wick theorem for a multiconfiguration reference wave function. Journal of Chemical Physics, 1997, 107, 432-449.	3.0	236
9	Molecular applications of multireference coupledâ€cluster methods using an incomplete model space: Direct calculation of excitation energies. Journal of Chemical Physics, 1988, 88, 4357-4366.	3.0	228
10	The linked-cluster theorem in the open-shell coupled-cluster theory for incomplete model spaces. Chemical Physics Letters, 1986, 125, 207-212.	2.6	211
11	State-Specific Multi-Reference Coupled Cluster Formulations: Two Paradigms. Advances in Quantum Chemistry, 1998, , 163-193.	0.8	172
12	Molecular Applications of a Size-Consistent State-Specific Multireference Perturbation Theory with Relaxed Model-Space Coefficients. Journal of Physical Chemistry A, 1999, 103, 1822-1830.	2.5	140
13	Aspects of linked cluster expansion in general model space many-body perturbation and coupled-cluster theory. International Journal of Quantum Chemistry, 1986, 30, 409-435.	2.0	122
14	Full implementation and benchmark studies of Mukherjeeâ€™s state-specific multireference coupled-cluster ansatz. Journal of Chemical Physics, 2010, 132, 074103.	3.0	114
15	Aspects of separability in the coupled cluster based direct methods for energy differences. Theoretica Chimica Acta, 1991, 80, 441-467.	0.8	113
16	On the hierarchy equations of the wave-operator for open-shell systems. Pramana - Journal of Physics, 1979, 12, 203-225.	1.8	104
17	A state-specific approach to multireference coupled electron-pair approximation like methods: Development and applications. Journal of Chemical Physics, 2004, 120, 5968-5986.	3.0	98
18	Development of a size-consistent state-specific multireference perturbation theory with relaxed model-space coefficients. Chemical Physics Letters, 1999, 299, 42-50.	2.6	92

#	Article	IF	Citations
19	The construction of a size-extensive intermediate Hamiltonian in a coupled-cluster framework. Chemical Physics Letters, 1992, 197, 236-242.	2.6	89
20	Size-extensive effective hamiltonian formalisms using quasi-Hilbert and quasi-Fock space strategies with incomplete model spaces. Chemical Physics Letters, 1989, 163, 171-177.	2.6	74
21	Application of linear response theory in a coupled cluster framework for the calculation of ionization potentials. Molecular Physics, 1981, 43, 173-179.	1.7	67
22	A companion perturbation theory for state-specific multireference coupled cluster methods. Physical Chemistry Chemical Physics, 2009, 11, 4728.	2.8	65
23	Comparison of low-order multireference many-body perturbation theories. Journal of Chemical Physics, 2005, 122, 134105.	3.0	62
24	Development of a linear response theory based on a state-specific multireference coupled cluster formalism. Journal of Chemical Physics, 2000, 112, 7939-7952.	3.0	55
25	Fock space multireference coupled cluster theory: noniterative inclusion of triples for excitation energies. Theoretical Chemistry Accounts, 1998, 99, 100-105.	1.4	54
26	Irreducible Brillouin conditions and contracted Schrol̂dinger equations for n-electron systems. II. Spin-free formulation. Journal of Chemical Physics, 2002, 116, 4787.	3.0	51
27	State-specific Multi-reference Perturbation Theories with Relaxed Coefficients: Molecular Applications. International Journal of Molecular Sciences, 2002, 3, 733-754.	4.1	49
28	Some aspects of self-consistent propagator theories. Physical Review A, 1985, 31, 1287-1298.	2.5	46
29	Property calculations using perturbed orbitals via state-specific multireference coupled-cluster and perturbation theories. Journal of Chemical Physics, 1999, 111, 3820-3831.	3.0	44
30	A spin-adapted size-extensive state-specific multi-reference perturbation theory. I. Formal developments. Journal of Chemical Physics, 2012, 136, 024105.	3.0	43
31	An explicitly spin-free compact open-shell coupled cluster theory using a multireference combinatoric exponential ansatz: Formal development and pilot applications. Journal of Chemical Physics, 2009, 131, 044124.	3.0	39
32	The spin-free analogue of Mukherjee's state-specific multireference coupled cluster theory. Journal of Chemical Physics, 2011, 134, 054122.	3.0	39
33	A hermitian open-shell many-body perturbation theory for treating intruder states. Pramana - Journal of Physics, 1984, 23, 651-664.	1.8	36
34	Unitary group adapted state-specific multi-reference coupled cluster theory: Formulation and pilot numerical applications. Journal of Chemical Physics, 2012, 137, 024105.	3.0	36
35	A spin-adapted size-extensive state-specific multi-reference perturbation theory with various partitioning schemes. II. Molecular applications. Journal of Chemical Physics, 2012, 136, 024106.	3.0	31
36	A study of the ionisation and excitation energies of core electrons using a unitary group adapted state universal approach. Molecular Physics, 2013, 111, 2625-2639.	1.7	27

#	Article	IF	Citations
37	Unitary coupled-cluster based self-consistent polarization propagator theory: A third-order formulation and pilot applications. Journal of Chemical Physics, 2018, 148, 244110.	3.0	27
38	4-Component relativistic calculations of L₃ionization and excitations for the isoelectronic species UO₂²⁺, OUN⁺and UN₂. Physical Chemistry Chemical Physics, 2016, 18, 21010-21023.	2.8	24
39	Timeâ€independent theory of oneâ€particle Greenâ€™s functions. Journal of Chemical Physics, 1989, 90, 5578-5594.	3.0	23
40	Consistent propagator theory based on the extended coupled-cluster parametrization of the ground state. Physical Review A, 1993, 47, 3632-3648.	2.5	23
41	Minimal parametrization of ann-electron state. Physical Review A, 2005, 71, .	2.5	23
42	Formulation and implementation of a unitary group adapted state universal multi-reference coupled cluster (UGA-SUMRCC) theory: Excited and ionized state energies. Journal of Chemical Physics, 2012, 137, 074104.	3.0	23
43	A universal explicit electron correlation correction applied to Mukherjeeâ€™s multi-reference perturbation theory. Chemical Physics Letters, 2012, 531, 247-251.	2.6	22
44	An Effective Liouvillean Formalism for Propagators in Fock Space: Connection with Effective Hamiltonian Approach for Energy Differences. Lecture Notes in Quantum Chemistry II, 1989, , 257-274.	0.3	22
45	Resolvent operator approach to manyâ€body perturbation theory. II. Open shells. Journal of Chemical Physics, 1982, 76, 1979-1994.	3.0	20
46	A FINITE-TEMPERATURE GENERALISATION OF THE COUPLED CLUSTER METHOD: A NON-PERTURBATIVE ACCESS TO GRAND PARTITION FUNCTIONS. International Journal of Modern Physics B, 2003, 17, 5367-5377.	2.0	18
47	A compact spinâ€free combinatoric openâ€shell coupled cluster theory applied to singleâ€reference doublets. International Journal of Quantum Chemistry, 2008, 108, 2211-2222.	2.0	18
48	Unitary group adapted state specific multireference perturbation theory: Formulation and pilot applications. Journal of Computational Chemistry, 2015, 36, 670-688.	3.3	18
49	Development and applications of a unitary group adapted state specific multi-reference coupled cluster theory with internally contracted treatment of inactive double excitations. Journal of Chemical Physics, 2012, 137, 094104.	3.0	15
50	Aspects of Size-Consistency of Orbitally Noninvariant Size-Extensive Multireference Perturbation Theories: A Case Study Using UGA-SSMRPT2 as a Prototype. Journal of Chemical Theory and Computation, 2015, 11, 4129-4145.	5.3	15
51	On estimates of the quantum recurrence time. Journal of Chemical Physics, 1986, 84, 3212-3214.	3.0	12
52	Development and applications of a relaxation-inducing cluster expansion theory for treating strong relaxation and differential correlation effects. Theoretical Chemistry Accounts, 1999, 102, 317-327.	1.4	12
53	Inclusion of orbital relaxation and correlation through the unitary group adapted open shell coupled cluster theory using non-relativistic and scalar relativistic Hamiltonians to study the core ionization potential of molecules containing light to medium-heavy elements. Journal of Chemical Physics, 2018, 148, 054107.	3.0	11
54	Orthonormality-constrained orbital optimisations in MC-SCF theory. Proceedings of the Indian Academy of Sciences - Section A, 1978, 87, 37-43.	0.2	11

#	Article	IF	Citations
55	Generalization of coupled-cluster response theory to multireference expansion spaces: application of the coupled-cluster singles and doubles effective Hamiltonian. Theoretical Chemistry Accounts, 1999, 102, 252-261.	1.4	9
56	Aspects of size extensivity in unitary group adapted multi-reference coupled cluster theories: the role of cumulant decomposition of spin-free reduced density matrices. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	9
57	On a new partitioning of the Hamiltonian in many-body calculation of pair-correlation energies in closed-shell systems. International Journal of Quantum Chemistry, 1975, 9, 545-554.	2.0	8
58	Resolvent operator approach to manyâ€body perturbation theory. I. Closed shells. Journal of Chemical Physics, 1982, 76, 1972-1978.	3.0	8
59	Resolvent operator approach to manyâ€body perturbation theory. III. Applications. Journal of Chemical Physics, 1982, 76, 1995-2002.	3.0	8
60	A hybrid technique of orthonormality constrained orbital optimization inSCF calculations. International Journal of Quantum Chemistry, 1981, 20, 1165-1177.	2.0	7
61	Communication: Extension of a universal explicit electron correlation correction to general complete active spaces. Journal of Chemical Physics, 2013, 138, 211101.	3.0	7
62	A comparative calculation on excited state energies of some conjugated hydrocarbons. International Journal of Quantum Chemistry, 1974, 8, 247-253.	2.0	6
63	Generalized Normal Ordering, Irreducible Brillouin Conditions, and Contracted SchrÃ¶dinger Equations. Advances in Chemical Physics, 2007, , 293-330.	0.3	6
64	Exploration of Various Aspects of UGA-SUMRCC: Size Extensivity, Possible Use of Sufficiency Conditions, and an Extension for Direct Determination of Energy Differences. Journal of Chemical Theory and Computation, 2013, 9, 2573-2590.	5.3	6
65	Orbital optimisation in single open-shell configurations: A sequential unconstrained minimisation technique. International Journal of Quantum Chemistry, 1975, 9, 943-949.	2.0	5
66	Convergence problems inSCF calculations: Further applications of a new technique based on the use of inverse Fock operator. International Journal of Quantum Chemistry, 1984, 25, 809-816.	2.0	4
67	Towards the Development and Applications of Manifestly Spin-free Multi-reference Coupled Electron-pair Approximation-like Methods: A State Specific Approach. Theoretical Chemistry Accounts, 2006, 116, 621-636.	1.4	3
68	Exploration of interlacing and avoided crossings in a manifold of potential energy curves by a unitary group adapted state specific multi-reference perturbation theory (UGA-SSMRPT). Journal of Chemical Physics, 2021, 155, 014101.	3.0	3
69	Symmetry-adapted many-body perturbation theory: use of the wave operator matrix elements. Pramana - Journal of Physics, 1979, 13, 535-544.	1.8	2
70	Recent advances in spin-free state-specific and state-universal multi-reference coupled cluster formalisms: A unitary group adapted approach. , 2012, , .		2
71	RESPONSE THEORIES BASED ON A STATE-SPECIFIC MULTI-REFERENCE COUPLED CLUSTER FORMALISM. Recent Advances in Computational, 1999, , 65-93.	0.8	1
72	Reappraisal of the normal ordered Jeziorski-Monkhorst ansatz in the UGA-OSCC theory for a study of IP, EA and EE. Molecular Physics, 2021, 119, .	1.7	1

#	Article	IF	Citations
73	A FINITE-TEMPERATURE GENERALISATION OF THE COUPLED CLUSTER METHOD: A NON-PERTURBATIVE ACCESS TO GRAND PARTITION FUNCTIONS. , 2002, , .		1
74	Applications of a Novel Spin-free Combinatoric Open-shell Coupled Cluster (COS-CC) Theory to Single-reference Doublets. AIP Conference Proceedings, 2007, , .	0.4	0
75	A compact spin-free coupled-cluster theory for open-shell systems. AIP Conference Proceedings, 2008, , .	0.4	0