# Debashis Mukherjee

List of Publications by Year
in descending order

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| 75 | 5,256 | 134610 | 97045 |
|---|---|---|---|
| papers | citations | 34 h-index | 71 g-index |

| 75 | 75 | 75 | 1148 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | 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. | 1.2 | 3 |
| 2 | 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, . | 0.8 | 1 |
| 3 | 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. | 1.2 | 11 |
| 4 | Unitary coupled-cluster based self-consistent polarization propagator theory: A third-order formulation and pilot applications. Journal of Chemical Physics, 2018, 148, 244110. | 1.2 | 27 |
| 5 | 4-Component relativistic calculations of L<sub>3</sub>ionization and excitations for the isoelectronic species UO<sub>2</sub><sup>2+</sup>, OUN<sup>+</sup>and UN<sub>2</sub>. Physical Chemistry Chemical Physics, 2016, 18, 21010-21023. | 1.3 | 24 |
| 6 | 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. | 2.3 | 15 |
| 7 | Unitary group adapted state specific multireference perturbation theory: Formulation and pilot applications. Journal of Computational Chemistry, 2015, 36, 670-688. | 1.5 | 18 |
| 8 | 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. | 0.5 | 9 |
| 9 | 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. | 2.3 | 6 |
| 10 | Communication: Extension of a universal explicit electron correlation correction to general complete active spaces. Journal of Chemical Physics, 2013, 138, 211101. | 1.2 | 7 |
| 11 | 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. | 0.8 | 27 |
| 12 | Unitary group adapted state-specific multi-reference coupled cluster theory: Formulation and pilot numerical applications. Journal of Chemical Physics, 2012, 137, 024105. | 1.2 | 36 |
| 13 | 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. | 1.2 | 15 |
| 14 | 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. | 1.2 | 23 |
| 15 | 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. | 1.2 | 31 |
| 16 | A spin-adapted size-extensive state-specific multi-reference perturbation theory. I. Formal developments. Journal of Chemical Physics, 2012, 136, 024105. | 1.2 | 43 |
| 17 | Recent advances in spin-free state-specific and state-universal multi-reference coupled cluster formalisms: A unitary group adapted approach. , 2012, , . | | 2 |
| 18 | A universal explicit electron correlation correction applied to Mukherjeeâ€™s multi-reference perturbation theory. Chemical Physics Letters, 2012, 531, 247-251. | 1.2 | 22 |

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|---|---|---|---|
| 19 | The spin-free analogue of Mukherjee's state-specific multireference coupled cluster theory. Journal of Chemical Physics, 2011, 134, 054122. | 1.2 | 39 |
| 20 | Full implementation and benchmark studies of Mukherjeeâ€™s state-specific multireference coupled-cluster ansatz. Journal of Chemical Physics, 2010, 132, 074103. | 1.2 | 114 |
| 21 | 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. | 1.2 | 39 |
| 22 | A companion perturbation theory for state-specific multireference coupled cluster methods. Physical Chemistry Chemical Physics, 2009, 11, 4728. | 1.3 | 65 |
| 23 | A compact spinâ€free combinatoric openâ€shell coupled cluster theory applied to singleâ€reference doublets. International Journal of Quantum Chemistry, 2008, 108, 2211-2222. | 1.0 | 18 |
| 24 | A compact spin-free coupled-cluster theory for open-shell systems. AIP Conference Proceedings, 2008, , . | 0.3 | 0 |
| 25 | Applications of a Novel Spin-free Combinatoric Open-shell Coupled Cluster (COS-CC) Theory to Single-reference Doublets. AIP Conference Proceedings, 2007, , . | 0.3 | 0 |
| 26 | Generalized Normal Ordering, Irreducible Brillouin Conditions, and Contracted SchrÃ¶dinger Equations. Advances in Chemical Physics, 2007, , 293-330. | 0.3 | 6 |
| 27 | 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. | 0.5 | 3 |
| 28 | Comparison of low-order multireference many-body perturbation theories. Journal of Chemical Physics, 2005, 122, 134105. | 1.2 | 62 |
| 29 | Minimal parametrization of ann-electron state. Physical Review A, 2005, 71, . | 1.0 | 23 |
| 30 | A state-specific approach to multireference coupled electron-pair approximation like methods: Development and applications. Journal of Chemical Physics, 2004, 120, 5968-5986. | 1.2 | 98 |
| 31 | 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. | 1.0 | 18 |
| 32 | Irreducible Brillouin conditions and contracted Schrol̂dinger equations for n-electron systems. II. Spin-free formulation. Journal of Chemical Physics, 2002, 116, 4787. | 1.2 | 51 |
| 33 | State-specific Multi-reference Perturbation Theories with Relaxed Coefficients: Molecular Applications. International Journal of Molecular Sciences, 2002, 3, 733-754. | 1.8 | 49 |
| 34 | A FINITE-TEMPERATURE GENERALISATION OF THE COUPLED CLUSTER METHOD: A NON-PERTURBATIVE ACCESS TO GRAND PARTITION FUNCTIONS. , 2002, , . | | 1 |
| 35 | Development of a linear response theory based on a state-specific multireference coupled cluster formalism. Journal of Chemical Physics, 2000, 112, 7939-7952. | 1.2 | 55 |
| 36 | RESPONSE THEORIES BASED ON A STATE-SPECIFIC MULTI-REFERENCE COUPLED CLUSTER FORMALISM. Recent Advances in Computational, 1999, , 65-93. | 0.8 | 1 |

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|---|---|---|---|
| 37 | Property calculations using perturbed orbitals via state-specific multireference coupled-cluster and perturbation theories. Journal of Chemical Physics, 1999, 111, 3820-3831. | 1.2 | 44 |
| 38 | Cumulant expansion of the reduced density matrices. Journal of Chemical Physics, 1999, 110, 2800-2809. | 1.2 | 241 |
| 39 | A size-consistent state-specific multireference coupled cluster theory: Formal developments and molecular applications. Journal of Chemical Physics, 1999, 110, 6171-6188. | 1.2 | 393 |
| 40 | Development of a size-consistent state-specific multireference perturbation theory with relaxed model-space coefficients. Chemical Physics Letters, 1999, 299, 42-50. | 1.2 | 92 |
| 41 | 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. | 0.5 | 9 |
| 42 | 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. | 0.5 | 12 |
| 43 | 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. | 1.1 | 140 |
| 44 | Fock space multireference coupled cluster theory: noniterative inclusion of triples for excitation energies. Theoretical Chemistry Accounts, 1998, 99, 100-105. | 0.5 | 54 |
| 45 | State-Specific Multi-Reference Coupled Cluster Formulations: Two Paradigms. Advances in Quantum Chemistry, 1998, , 163-193. | 0.4 | 172 |
| 46 | Normal order and extended Wick theorem for a multiconfiguration reference wave function. Journal of Chemical Physics, 1997, 107, 432-449. | 1.2 | 236 |
| 47 | Consistent propagator theory based on the extended coupled-cluster parametrization of the ground state. Physical Review A, 1993, 47, 3632-3648. | 1.0 | 23 |
| 48 | The construction of a size-extensive intermediate Hamiltonian in a coupled-cluster framework. Chemical Physics Letters, 1992, 197, 236-242. | 1.2 | 89 |
| 49 | Aspects of separability in the coupled cluster based direct methods for energy differences. Theoretica Chimica Acta, 1991, 80, 441-467. | 0.9 | 113 |
| 50 | Use of Cluster Expansion Methods in the Open-Shell Correlation Problem. Advances in Quantum Chemistry, 1989, 20, 291-373. | 0.4 | 353 |
| 51 | Size-extensive effective hamiltonian formalisms using quasi-Hilbert and quasi-Fock space strategies with incomplete model spaces. Chemical Physics Letters, 1989, 163, 171-177. | 1.2 | 74 |
| 52 | Timeâ€independent theory of oneâ€particle Greenâ€™s functions. Journal of Chemical Physics, 1989, 90, 5578-5594. | 1.2 | 23 |
| 53 | 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 |
| 54 | 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. | 1.2 | 228 |

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|---|---|---|---|
| 55 | On the connectivity criteria in the open-shell coupled-cluster theory for general model spaces. Physics Reports, 1987, 151, 93-127. | 10.3 | 453 |
| 56 | The linked-cluster theorem in the open-shell coupled-cluster theory for incomplete model spaces. Chemical Physics Letters, 1986, 125, 207-212. | 1.2 | 211 |
| 57 | 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. | 1.0 | 122 |
| 58 | On estimates of the quantum recurrence time. Journal of Chemical Physics, 1986, 84, 3212-3214. | 1.2 | 12 |
| 59 | Some aspects of self-consistent propagator theories. Physical Review A, 1985, 31, 1287-1298. | 1.0 | 46 |
| 60 | Application of cluster expansion techniques to open shells: Calculation of difference energies. Journal of Chemical Physics, 1984, 80, 5058-5069. | 1.2 | 283 |
| 61 | A hermitian open-shell many-body perturbation theory for treating intruder states. Pramana - Journal of Physics, 1984, 23, 651-664. | 0.9 | 36 |
| 62 | 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. | 1.0 | 4 |
| 63 | Resolvent operator approach to manyâ€body perturbation theory. I. Closed shells. Journal of Chemical Physics, 1982, 76, 1972-1978. | 1.2 | 8 |
| 64 | Resolvent operator approach to manyâ€body perturbation theory. II. Open shells. Journal of Chemical Physics, 1982, 76, 1979-1994. | 1.2 | 20 |
| 65 | Resolvent operator approach to manyâ€body perturbation theory. III. Applications. Journal of Chemical Physics, 1982, 76, 1995-2002. | 1.2 | 8 |
| 66 | Application of linear response theory in a coupled cluster framework for the calculation of ionization potentials. Molecular Physics, 1981, 43, 173-179. | 0.8 | 67 |
| 67 | A hybrid technique of orthonormality constrained orbital optimization inSCF calculations. International Journal of Quantum Chemistry, 1981, 20, 1165-1177. | 1.0 | 7 |
| 68 | Symmetry-adapted many-body perturbation theory: use of the wave operator matrix elements. Pramana - Journal of Physics, 1979, 13, 535-544. | 0.9 | 2 |
| 69 | On the hierarchy equations of the wave-operator for open-shell systems. Pramana - Journal of Physics, 1979, 12, 203-225. | 0.9 | 104 |
| 70 | Orthonormality-constrained orbital optimisations in MC-SCF theory. Proceedings of the Indian Academy of Sciences - Section A, 1978, 87, 37-43. | 0.2 | 11 |
| 71 | 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. | 0.8 | 281 |
| 72 | 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. | 1.0 | 8 |

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|---|---|---|---|
| 73 | Orbital optimisation in single open-shell configurations: A sequential unconstrained minimisation technique. International Journal of Quantum Chemistry, 1975, 9, 943-949. | 1.0 | 5 |
| 74 | Correlation problem in open-shell atoms and molecules. Molecular Physics, 1975, 30, 1861-1888. | 0.8 | 282 |
| 75 | A comparative calculation on excited state energies of some conjugated hydrocarbons. International Journal of Quantum Chemistry, 1974, 8, 247-253. | 1.0 | 6 |