Dipayan Datta

List of Publications by Year in descending order

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23 papers	1,285 citations	687363 13 h-index	677142 22 g-index
24 all docs	24 docs citations	24 times ranked	1101 citing authors

#	Article	IF	Citations
1	Recent developments in the general atomic and molecular electronic structure system. Journal of Chemical Physics, 2020, 152, 154102.	3.0	734
2	A state-specific partially internally contracted multireference coupled cluster approach. Journal of Chemical Physics, 2011, 134, 214116.	3.0	74
3	Multireference equation-of-motion coupled cluster theory. Journal of Chemical Physics, 2012, 137, 204107.	3.0	62
4	Analytic energy derivatives for the calculation of the first-order molecular properties using the domain-based local pair-natural orbital coupled-cluster theory. Journal of Chemical Physics, 2016, 145, .	3.0	57
5	Comparative study of multireference perturbative theories for ground and excited states. Journal of Chemical Physics, 2009, 131, 204104.	3.0	51
6	Communication: Multireference equation of motion coupled cluster: A transform and diagonalize approach to electronic structure. Journal of Chemical Physics, 2014, 140, 081102.	3.0	44
7	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
8	The spin-free analogue of Mukherjee's state-specific multireference coupled cluster theory. Journal of Chemical Physics, 2011, 134, 054122.	3.0	39
9	Additional global internal contraction in variations of multireference equation of motion coupled cluster theory. Journal of Chemical Physics, 2013, 138, 134108.	3.0	33
10	A Massively Parallel Implementation of the CCSD(T) Method Using the Resolution-of-the-Identity Approximation and a Hybrid Distributed/Shared Memory Parallelization Model. Journal of Chemical Theory and Computation, 2021, 17, 4799-4822.	5.3	23
11	Development and pilot molecular applications of the uncoupled state-specific MRCC (UC-SS-MRCC) theory. Chemical Physics, 2008, 349, 115-120.	1.9	20
12	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
13	A Non-antisymmetric Tensor Contraction Engine for the Automated Implementation of Spin-Adapted Coupled Cluster Approaches. Journal of Chemical Theory and Computation, 2013, 9, 2639-2653.	5.3	16
14	Inactive excitations in Mukherjee's state-specific multireference coupled cluster theory treated with internal contraction: Development and applications. Journal of Chemical Physics, 2012, 136, 164104.	3.0	13
15	Communication: Spin densities within a unitary group based spin-adapted open-shell coupled-cluster theory: Analytic evaluation of isotropic hyperfine-coupling constants for the combinatoric open-shell coupled-cluster scheme. Journal of Chemical Physics, 2015, 143, 011101.	3.0	13
16	Accurate Prediction of Hyperfine Coupling Tensors for Main Group Elements Using a Unitary Group Based Rigorously Spin-Adapted Coupled-Cluster Theory. Journal of Chemical Theory and Computation, 2019, 15, 1572-1592.	5.3	12
17	Analytic first derivatives for a spin-adapted open-shell coupled cluster theory: Evaluation of first-order electrical properties. Journal of Chemical Physics, 2014, 141, 104102.	3.0	10
18	A novel VU-MRCC formalism for the simultaneous treatment of strong relaxation and correlation effects with applications to electron affinity of neutral radicals. Chemical Physics, 2006, 329, 290-306.	1.9	9

#	Article	IF	Citations
19	Use of a convenient size-extensive normalization in multi-reference coupled cluster (MRCC) theory with incomplete model space: A novel valence universal MRCC formulation. Chemical Physics, 2009, 356, 54-63.	1.9	8
20	57Fe MÃ¶ssbauer parameters from domain based local pair-natural orbital coupled-cluster theory. Journal of Chemical Physics, 2020, 153, 204101.	3.0	5
21	PDG: A Composite Method Based on the Resolution of the Identity. Journal of Physical Chemistry A, 2021, 125, 9421-9429.	2.5	3
22	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
23	A compact spin-free coupled-cluster theory for open-shell systems. AIP Conference Proceedings, 2008, , .	0.4	0