Dipayan Datta

List of Publications by Year in descending order

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Version: 2024-02-01

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	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
2	PDG: A Composite Method Based on the Resolution of the Identity. Journal of Physical Chemistry A, 2021, 125, 9421-9429.	2.5	3
3	57Fe MÃ¶ssbauer parameters from domain based local pair-natural orbital coupled-cluster theory. Journal of Chemical Physics, 2020, 153, 204101.	3.0	5
4	Recent developments in the general atomic and molecular electronic structure system. Journal of Chemical Physics, 2020, 152, 154102.	3.0	734
5	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
6	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
7	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
8	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
9	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
10	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
11	Additional global internal contraction in variations of multireference equation of motion coupled cluster theory. Journal of Chemical Physics, 2013, 138, 134108.	3.0	33
12	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
13	Multireference equation-of-motion coupled cluster theory. Journal of Chemical Physics, 2012, 137, 204107.	3.0	62
14	The spin-free analogue of Mukherjee's state-specific multireference coupled cluster theory. Journal of Chemical Physics, 2011, 134, 054122.	3.0	39
15	A state-specific partially internally contracted multireference coupled cluster approach. Journal of Chemical Physics, 2011, 134, 214116.	3.0	74
16	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
17	Comparative study of multireference perturbative theories for ground and excited states. Journal of Chemical Physics, 2009, 131, 204104.	3.0	51
18	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

#	Article	IF	Citations
19	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
20	Development and pilot molecular applications of the uncoupled state-specific MRCC (UC-SS-MRCC) theory. Chemical Physics, 2008, 349, 115-120.	1.9	20
21	A compact spin-free coupled-cluster theory for open-shell systems. AIP Conference Proceedings, 2008, , .	0.4	0
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 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