Jun Shen

List of Publications by Year
in descending order

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39	1,882	361296 20	302012 39
papers	citations	h-index	g-index

40	40	40	1629
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Recent developments in the general atomic and molecular electronic structure system. Journal of Chemical Physics, 2020, 152, 154102.	1.2	734
2	An efficient implementation of the â€œcluster-in-moleculeâ€•approach for local electron correlation calculations. Journal of Chemical Physics, 2006, 125, 074109.	1.2	126
3	The Ground State Electronic Energy of Benzene. Journal of Physical Chemistry Letters, 2020, 11, 8922-8929.	2.1	90
4	Converging High-Level Coupled-Cluster Energetics by MonteÂCarlo Sampling and Moment Expansions. Physical Review Letters, 2017, 119, 223003.	2.9	73
5	Doubly electron-attached and doubly ionized equation-of-motion coupled-cluster methods with 4-particleâ€“2-hole and 4-holeâ€“2-particle excitations and their active-space extensions. Journal of Chemical Physics, 2013, 138, 194102.	1.2	71
6	Biorthogonal moment expansions in coupled-cluster theory: Review of key concepts and merging the renormalized and active-space coupled-cluster methods. Chemical Physics, 2012, 401, 180-202.	0.9	69
7	Communication: Approaching exact quantum chemistry by cluster analysis of full configuration interaction quantum Monte Carlo wave functions. Journal of Chemical Physics, 2018, 149, 151101.	1.2	62
8	Combining active-space coupled-cluster methods with moment energy corrections via the CC(P;Q) methodology, with benchmark calculations for biradical transition states. Journal of Chemical Physics, 2012, 136, 144104.	1.2	61
9	Photoluminescence, photophysics, and photochemistry of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mrow><mml:msub><mml:mi mathvariant="normal">V</mml:mi><mml:mi mathvariant="normal">B</mml:mi></mml:msub></mml:mrow><mml:mo>â^’</mml:mo></mml:msup></mml:math> defect in hexagonal boron nitride. Physical Review B, 2020, 102, .	1.1	60
10	Merging Active-Space and Renormalized Coupled-Cluster Methods via the CC(P;Q) Formalism, with Benchmark Calculations for Singletâ€“Triplet Gaps in Biradical Systems. Journal of Chemical Theory and Computation, 2012, 8, 4968-4988.	2.3	53
11	Block correlated coupled cluster method with a complete-active-space self-consistent-field reference function: The formula for general active spaces and its applications for multibond breaking systems. Journal of Chemical Physics, 2008, 128, 224107.	1.2	41
12	Combining active-space coupled-cluster approaches with moment energy corrections via the CC(P;Q) methodology: connected quadruple excitations. Molecular Physics, 2017, 115, 2860-2891.	0.8	35
13	Geometries, Binding Energies, Ionization Potentials, and Electron Affinities of Metal Clusters: Mg_n^{0,ÂÂ±Â1}, n = 1â€“7. Journal of Physical Chemistry C, 2016, 120, 13275-13286.	1.5	32
14	Performance of Block Correlated Coupled Cluster Method with the CASSCF Reference Function for the Prediction of Activation Barriers, Spectroscopic Constants in Diatomic Molecules, and Singletâ^’Triplet Gaps in Diradicals. Journal of Physical Chemistry A, 2008, 112, 12518-12525.	1.1	29
15	Accurate excited-state energetics by a combination of Monte Carlo sampling and equation-of-motion coupled-cluster computations. Journal of Chemical Physics, 2019, 150, 111101.	1.2	28
16	Block correlated coupled cluster method with the complete active-space self-consistent-field reference function: Applications for low-lying electronic excited states. Journal of Chemical Physics, 2009, 131, 174101.	1.2	27
17	Application of the CC(P;Q) Hierarchy of Coupled-Cluster Methods to the Beryllium Dimer. Journal of Physical Chemistry A, 2018, 122, 1350-1368.	1.1	27
18	Spectroscopic Constants of Single-Bond Diatomic Molecules and Singletâ^’Triplet Gaps of Diradicals by the Block-Correlated Coupled Cluster Theory. Journal of Physical Chemistry A, 2008, 112, 4703-4709.	1.1	24

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19	A coupled cluster approach with a hybrid treatment of connected triple excitations for bond-breaking potential energy surfaces. Journal of Chemical Physics, 2010, 132, 114115.	1.2	22
20	Doubly electron-attached and doubly ionised equation-of-motion coupled-cluster methods withÂfull and active-space treatments of 4-particleâ€“2-hole and 4-holeâ€“2-particle excitations: the role ofÂorbital choices. Molecular Physics, 2014, 112, 868-885.	0.8	21
21	Systematic design of active spaces for multi-reference calculations of singletâ€“triplet gaps of organic diradicals, with benchmarks against doubly electron-attached coupled-cluster data. Journal of Chemical Physics, 2017, 147, 164120.	1.2	20
22	New coupled cluster approaches based on the unrestricted Hartreeâ€“Fock reference for treating molecules with multireference character. Physical Chemistry Chemical Physics, 2011, 13, 8795.	1.3	16
23	Intricacies of van der Waals Interactions in Systems with Elongated Bonds Revealed by Electron-Groups Embedding and High-Level Coupled-Cluster Approaches. Journal of Chemical Theory and Computation, 2017, 13, 5404-5419.	2.3	16
24	A coupled cluster approach with a hybrid treatment of connected triple excitations: Implementation and applications for open-shell systems. Journal of Chemical Physics, 2010, 133, 234106.	1.2	15
25	The coupled cluster approach with a hybrid treatment of connected triple excitations based on the restricted Hartreeâ€“Fock reference. Journal of Chemical Physics, 2011, 134, 044134.	1.2	15
26	Economical Doubly Electron-Attached Equation-of-Motion Coupled-Cluster Methods with an Active-Space Treatment of Three-Particleâ€“One-Hole and Four-Particleâ€“Two-Hole Excitations. Journal of Physical Chemistry A, 2017, 121, 3469-3485.	1.1	14
27	Is Externally Corrected Coupled Cluster Always Better Than the Underlying Truncated Configuration Interaction?. Journal of Chemical Theory and Computation, 2021, 17, 4006-4027.	2.3	14
28	Internal Conversion between Bright (1¹B_u⁺) and Dark (2¹A_g^{â€“}) States in s-trans-Butadiene and s-trans-Hexatriene. Journal of Physical Chemistry Letters, 2021, 12, 9720-9729.	2.1	14
29	High-level coupled-cluster energetics by Monte Carlo sampling and moment expansions: Further details and comparisons. Journal of Chemical Physics, 2021, 154, 124103.	1.2	12
30	Application of the coupled-cluster CC(P;Q) approaches to the magnesium dimer. Molecular Physics, 2019, 117, 1486-1506.	0.8	11
31	Accelerating convergence of equation-of-motion coupled-cluster computations using the semi-stochastic CC(P;Q) formalism. Molecular Physics, 2020, 118, e1817592.	0.8	11
32	High-level coupled-cluster energetics by merging moment expansions with selected configuration interaction. Journal of Chemical Physics, 2021, 155, 174114.	1.2	10
33	Double electron-attachment equation-of-motion coupled-cluster methods with up to 4-particleâ€“2-hole excitations: improved implementation and application to singletâ€“triplet gaps in ortho- , meta- , and para- benzyne isomers. Molecular Physics, 2021, 119, .	0.8	7
34	Singlet-triplet gaps in substituted carbenes predicted from block-correlated coupled cluster method. Science in China Series B: Chemistry, 2008, 51, 1197-1202.	0.8	6
35	Addressing strong correlation by approximate coupled-pair methods with active-space and full treatments of three-body clusters. Molecular Physics, 2022, 120, .	0.8	5
36	Isoenergetic two-photon excitation enhances solvent-to-solute excited-state proton transfer. Journal of Chemical Physics, 2020, 153, 224301.	1.2	4

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37	The coupled cluster singles, doubles, and a hybrid treatment of connected triples based on the split virtual orbitals. Journal of Chemical Physics, 2012, 136, 044101.	1.2	3
38	Ab initiocoupled-cluster and multi-reference configuration interaction studies of the low-lying electronic states of 1,2,3,4-cyclobutanetetraone. Molecular Physics, 2016, 114, 695-708.	0.8	3
39	Comparison of some multireference electronic structure methods in illustrative applications. Science China Chemistry, 2010, 53, 289-296.	4.2	1