Zhendong Li

List of Publications by Year
in descending order

48 papers	3,131 citations	172457 29 h-index	233421 45 g-index
49 all docs	49 docs citations	49 times ranked	2269 citing authors

#	Article	IF	Citations
1	Effect of geometric configuration on compression behavior of 3D-printed polymeric triply periodic minimal surface sheets. Mechanics of Advanced Materials and Structures, 2023, 30, 2304-2314.	2.6	11
2	One-pot synthesis of N-doped carbon intercalated molybdenum disulfide nanohybrid for enhanced adsorption of tetracycline from aqueous solutions. Science of the Total Environment, 2021, 754, 141925.	8.0	34
3	Expressibility of comb tensor network states (CTNS) for the P-cluster and the FeMo-cofactor of nitrogenase. Electronic Structure, 2021, 3, 014001.	2.8	9
4	Low rank representations for quantum simulation of electronic structure. Npj Quantum Information, 2021, 7, .	6.7	54
5	Compressive behaviors of fractal-like honeycombs with different array configurations under low velocity impact loading. Thin-Walled Structures, 2021, 163, 107759.	5.3	47
6	Structured eigenvalue problems in electronic structure methods from a unified perspective. Chinese Journal of Chemical Physics, 2021, 34, 525-531.	1.3	1
7	Theoretical and numerical analysis of the folding mechanism of vertex-based hierarchical honeycomb structure. Mechanics of Advanced Materials and Structures, 2020, 27, 789-799.	2.6	30
8	Recent developments in the P<scp>y</scp>SCF program package. Journal of Chemical Physics, 2020, 153, 024109.	3.0	388
9	Analytic energy gradients of spin-adapted open-shell time-dependent density functional theory. Journal of Chemical Physics, 2020, 153, 164109.	3.0	20
10	Theoretical and numerical analyses on mechanical performance of octagonal honeycomb structures subjected to out-of-plane compression. Mechanics of Advanced Materials and Structures, 2020, 27, 1461-1472.	2.6	20
11	BDF: A relativistic electronic structure program package. Journal of Chemical Physics, 2020, 152, 064113.	3.0	79
12	Quantum computation of molecular response properties. Physical Review Research, 2020, 2, .	3.6	20
13	Generalization of the exponential basis for tensor network representations of long-range interactions in two and three dimensions. Physical Review B, 2019, 100, .	3.2	9
14	Stimulated X-ray Raman and Absorption Spectroscopy of Ironâ€“Sulfur Dimers. Journal of Physical Chemistry Letters, 2019, 10, 6664-6671.	4.6	8
15	Electronic landscape of the P-cluster of nitrogenase as revealed through many-electron quantum wavefunction simulations. Nature Chemistry, 2019, 11, 1026-1033.	13.6	67
16	Unraveling the Emission Mechanism of Radical-Based Organic Light-Emitting Diodes. Journal of Physical Chemistry Letters, 2019, 10, 574-580.	4.6	35
17	Stochastic many-body perturbation theory for electron correlation energies. Journal of Chemical Physics, 2019, 151, 244114.	3.0	9
18	Applying facilely synthesized CuO/CeO₂ photocatalyst to accelerate methylene blue degradation in hypersaline wastewater. Surface and Interface Analysis, 2019, 51, 336-344.	1.8	17

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19	The electronic complexity of the ground-state of the FeMo cofactor of nitrogenase as relevant to quantum simulations. Journal of Chemical Physics, 2019, 150, 024302.	3.0	59
20	P<scp>y</scp>SCF: the Pythonâ€based simulations of chemistry framework. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1340.	14.6	894
21	Efficient representation of long-range interactions in tensor network algorithms. Physical Review B, 2018, 98, .	3.2	11
22	A Perturbative Density Matrix Renormalization Group Algorithm for Large Active Spaces. Journal of Chemical Theory and Computation, 2018, 14, 4063-4071.	5.3	32
23	Communication: An efficient stochastic algorithm for the perturbative density matrix renormalization group in large active spaces. Journal of Chemical Physics, 2018, 148, 221104.	3.0	19
24	Combining the spin-separated exact two-component relativistic Hamiltonian with the equation-of-motion coupled-cluster method for the treatment of spinâ€“orbit splittings of light and heavy elements. Physical Chemistry Chemical Physics, 2017, 19, 3713-3721.	2.8	36
25	Spin-Projected Matrix Product States: Versatile Tool for Strongly Correlated Systems. Journal of Chemical Theory and Computation, 2017, 13, 2681-2695.	5.3	34
26	Performance of TD-DFT for Excited States of Open-Shell Transition Metal Compounds. Journal of Physical Chemistry A, 2017, 121, 3929-3942.	2.5	31
27	Time-Step Targeting Time-Dependent and Dynamical Density Matrix Renormalization Group Algorithms with ab Initio Hamiltonians. Journal of Chemical Theory and Computation, 2017, 13, 5560-5571.	5.3	45
28	Spin Separation of Relativistic Hamiltonians. , 2017, , 411-447.		6
29	Basic Structures of RelativisticWave Functions. , 2017, , 481-496.		5
30	Coalescence Conditions of Relativistic Wave Functions. , 2017, , 497-530.		2
31	Relativistic Explicit Correlation: Problemsand Solutions. , 2017, , 531-545.		4
32	Matrix product operators, matrix product states, and ab initio density matrix renormalization group algorithms. Journal of Chemical Physics, 2016, 145, 014102.	3.0	121
33	Hilbert space renormalization for the many-electron problem. Journal of Chemical Physics, 2016, 144, 084103.	3.0	5
34	Critical Assessment of Time-Dependent Density Functional Theory for Excited States of Open-Shell Systems: II. Doublet-Quartet Transitions. Journal of Chemical Theory and Computation, 2016, 12, 2517-2527.	5.3	21
35	Critical Assessment of TD-DFT for Excited States of Open-Shell Systems: I. Doubletâ€“Doublet Transitions. Journal of Chemical Theory and Computation, 2016, 12, 238-260.	5.3	35
36	Solvent Effects on the Optical Spectra and Excited-State Decay of Triphenylamine-thiadiazole with Hybridized Local Excitation and Intramolecular Charge Transfer. Journal of Physical Chemistry A, 2015, 119, 5233-5240.	2.5	73

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37	On the spin separation of algebraic two-component relativistic Hamiltonians: Molecular properties. Journal of Chemical Physics, 2014, 141, 054111.	3.0	67
38	First order nonadiabatic coupling matrix elements between excited states: Implementation and application at the TD-DFT and pp-TDA levels. Journal of Chemical Physics, 2014, 141, 244105.	3.0	74
39	Localization of Molecular Orbitals: From Fragments to Molecule. Accounts of Chemical Research, 2014, 47, 2758-2767.	15.6	34
40	First-order nonadiabatic coupling matrix elements between excited states: A Lagrangian formulation at the CIS, RPA, TD-HF, and TD-DFT levels. Journal of Chemical Physics, 2014, 141, 014110.	3.0	83
41	Combining spin-adapted open-shell TD-DFT with spinâ€“orbit coupling. Molecular Physics, 2013, 111, 3741-3755.	1.7	85
42	On the spin separation of algebraic two-component relativistic Hamiltonians. Journal of Chemical Physics, 2012, 137, 154114.	3.0	123
43	Relativistic explicit correlation: Coalescence conditions and practical suggestions. Journal of Chemical Physics, 2012, 136, 144117.	3.0	36
44	Theoretical and numerical assessments of spin-flip time-dependent density functional theory. Journal of Chemical Physics, 2012, 136, 024107.	3.0	66
45	Linear-Scaling Time-Dependent Density Functional Theory Based on the Idea of â€œFrom Fragments to Moleculeâ€• Journal of Chemical Theory and Computation, 2011, 7, 3643-3660.	5.3	70
46	Spin-adapted open-shell time-dependent density functional theory. II. Theory and pilot application. Journal of Chemical Physics, 2011, 134, 134101.	3.0	68
47	Spin-adapted open-shell time-dependent density functional theory. III. An even better and simpler formulation. Journal of Chemical Physics, 2011, 135, 194106.	3.0	57
48	Spin-adapted open-shell random phase approximation and time-dependent density functional theory. I. Theory. Journal of Chemical Physics, 2010, 133, 064106.	3.0	68