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	P<scp>y</scp>SCF: the Pythonâ€based simulations of chemistry framework. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1340.	14.6	894
2	Recent developments in the P<scp>y</scp>SCF program package. Journal of Chemical Physics, 2020, 153, 024109.	3.0	388
3	On the spin separation of algebraic two-component relativistic Hamiltonians. Journal of Chemical Physics, 2012, 137, 154114.	3.0	123
4	Matrix product operators, matrix product states, and ab initio density matrix renormalization group algorithms. Journal of Chemical Physics, 2016, 145, 014102.	3.0	121
5	Combining spin-adapted open-shell TD-DFT with spinâ€“orbit coupling. Molecular Physics, 2013, 111, 3741-3755.	1.7	85
6	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
7	BDF: A relativistic electronic structure program package. Journal of Chemical Physics, 2020, 152, 064113.	3.0	79
8	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
9	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
10	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
11	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
12	Spin-adapted open-shell time-dependent density functional theory. II. Theory and pilot application. Journal of Chemical Physics, 2011, 134, 134101.	3.0	68
13	On the spin separation of algebraic two-component relativistic Hamiltonians: Molecular properties. Journal of Chemical Physics, 2014, 141, 054111.	3.0	67
14	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
15	Theoretical and numerical assessments of spin-flip time-dependent density functional theory. Journal of Chemical Physics, 2012, 136, 024107.	3.0	66
16	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
17	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
18	Low rank representations for quantum simulation of electronic structure. Npj Quantum Information, 2021, 7, .	6.7	54

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19	Compressive behaviors of fractal-like honeycombs with different array configurations under low velocity impact loading. Thin-Walled Structures, 2021, 163, 107759.	5.3	47
20	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
21	Relativistic explicit correlation: Coalescence conditions and practical suggestions. Journal of Chemical Physics, 2012, 136, 144117.	3.0	36
22	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
23	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
24	Unraveling the Emission Mechanism of Radical-Based Organic Light-Emitting Diodes. Journal of Physical Chemistry Letters, 2019, 10, 574-580.	4.6	35
25	Localization of Molecular Orbitals: From Fragments to Molecule. Accounts of Chemical Research, 2014, 47, 2758-2767.	15.6	34
26	Spin-Projected Matrix Product States: Versatile Tool for Strongly Correlated Systems. Journal of Chemical Theory and Computation, 2017, 13, 2681-2695.	5.3	34
27	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
28	A Perturbative Density Matrix Renormalization Group Algorithm for Large Active Spaces. Journal of Chemical Theory and Computation, 2018, 14, 4063-4071.	5.3	32
29	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
30	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
31	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
32	Analytic energy gradients of spin-adapted open-shell time-dependent density functional theory. Journal of Chemical Physics, 2020, 153, 164109.	3.0	20
33	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
34	Quantum computation of molecular response properties. Physical Review Research, 2020, 2, .	3.6	20
35	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
36	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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37	Efficient representation of long-range interactions in tensor network algorithms. Physical Review B, 2018, 98, .	3.2	11
38	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
39	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
40	Stochastic many-body perturbation theory for electron correlation energies. Journal of Chemical Physics, 2019, 151, 244114.	3.0	9
41	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
42	Stimulated X-ray Raman and Absorption Spectroscopy of Ironâ€“Sulfur Dimers. Journal of Physical Chemistry Letters, 2019, 10, 6664-6671.	4.6	8
43	Spin Separation of Relativistic Hamiltonians. , 2017, , 411-447.		6
44	Hilbert space renormalization for the many-electron problem. Journal of Chemical Physics, 2016, 144, 084103.	3.0	5
45	Basic Structures of RelativisticWave Functions. , 2017, , 481-496.		5
46	Relativistic Explicit Correlation: Problemsand Solutions. , 2017, , 531-545.		4
47	Coalescence Conditions of Relativistic Wave Functions. , 2017, , 497-530.		2
48	Structured eigenvalue problems in electronic structure methods from a unified perspective. Chinese Journal of Chemical Physics, 2021, 34, 525-531.	1.3	1