Qiming Sun

List of Publications by Year
in descending order

25 papers	3,292 citations	304743 22 h-index	580821 25 g-index
25 all docs	25 docs citations	25 times ranked	2175 citing authors

#	Article	IF	Citations
1	Efficient evaluation of the Breit operator in the Pauli spinor basis. Journal of Chemical Physics, 2022, 157, .	3.0	14
2	Transfer learning with graph neural networks for optoelectronic properties of conjugated oligomers. Journal of Chemical Physics, 2021, 154, 024906.	3.0	28
3	Recent developments in the P<scp>y</scp>SCF program package. Journal of Chemical Physics, 2020, 153, 024109.	3.0	388
4	Machine learning Frenkel Hamiltonian parameters to accelerate simulations of exciton dynamics. Journal of Chemical Physics, 2020, 153, 074111.	3.0	20
5	OpenFermion: the electronic structure package for quantum computers. Quantum Science and Technology, 2020, 5, 034014.	5.8	214
6	Deep Learning for Optoelectronic Properties of Organic Semiconductors. Journal of Physical Chemistry C, 2020, 124, 7048-7060.	3.1	35
7	BDF: A relativistic electronic structure program package. Journal of Chemical Physics, 2020, 152, 064113.	3.0	79
8	Electronic structure of bulk manganese oxide and nickel oxide from coupled cluster theory. Physical Review B, 2020, 101, .	3.2	27
9	Ground-state phase diagram of the three-band Hubbard model from density matrix embedding theory. Physical Review Research, 2020, 2, .	3.6	22
10	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
11	P<scp>y</scp>SCF: the Pythonâ€based simulations of chemistry framework. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1340.	14.6	894
12	Gaussian-Based Coupled-Cluster Theory for the Ground-State and Band Structure of Solids. Journal of Chemical Theory and Computation, 2017, 13, 1209-1218.	5.3	171
13	A general second order complete active space self-consistent-field solver for large-scale systems. Chemical Physics Letters, 2017, 683, 291-299.	2.6	84
14	Towards the Solution of the Many-Electron Problem in Real Materials: Equation of State of the Hydrogen Chain with State-of-the-Art Many-Body Methods. Physical Review X, 2017, 7, .	8.9	171
15	Automated Construction of Molecular Active Spaces from Atomic Valence Orbitals. Journal of Chemical Theory and Computation, 2017, 13, 4063-4078.	5.3	119
16	Gaussian and plane-wave mixed density fitting for periodic systems. Journal of Chemical Physics, 2017, 147, 164119.	3.0	66
17	A Practical Guide to Density Matrix Embedding Theory in Quantum Chemistry. Journal of Chemical Theory and Computation, 2016, 12, 2706-2719.	5.3	147
18	Quantum Embedding Theories. Accounts of Chemical Research, 2016, 49, 2705-2712.	15.6	200

#	Article	IF	Citations
19	N-Electron Valence State Perturbation Theory Based on a Density Matrix Renormalization Group Reference Function, with Applications to the Chromium Dimer and a Trimer Model of Poly(p-Phenylenevinylene). Journal of Chemical Theory and Computation, 2016, 12, 1583-1591.	5.3	145
20	Libcint: An efficient general integral library for Gaussian basis functions. Journal of Computational Chemistry, 2015, 36, 1664-1671.	3.3	123
21	Stochastic Multiconfigurational Self-Consistent Field Theory. Journal of Chemical Theory and Computation, 2015, 11, 5316-5325.	5.3	86
22	Exact and Optimal Quantum Mechanics/Molecular Mechanics Boundaries. Journal of Chemical Theory and Computation, 2014, 10, 3784-3790.	5.3	37
23	Exact two-component relativistic theory for NMR parameters: General formulation and pilot application. Journal of Chemical Physics, 2012, 137, 174105.	3.0	54
24	Fully relativistic theories and methods for NMR parameters. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	45
25	Exact two-component relativistic theory for nuclear magnetic resonance parameters. Journal of Chemical Physics, 2009, 131, 081101.	3.0	56