Shiwei Zhang

List of Publications by Year in Descending Order

82 papers	3,415 citations	33 h-index	57 g-index
88 ext. papers	4,065 ext. citations	5.3 avg, IF	5.68 L-index

#	Paper	IF	Citations
82	Ab initio calculations in atoms, molecules, and solids, treating spin-orbit coupling and electron interaction on an equal footing.. *Journal of Chemical Physics*, **2022**, 156, 014107	3.9	1
81	Constrained-path auxiliary-field quantum Monte Carlo for coupled electrons and phonons. *Physical Review B*, **2021**, 103,	3.3	3
80	Tracking the Footprints of Spin Fluctuations: A MultiMethod, MultiMessenger Study of the Two-Dimensional Hubbard Model. *Physical Review X*, **2021**, 11,	9.1	24
79	Pseudo-BCS wave function from density matrix decomposition: Application in auxiliary-field quantum Monte Carlo. *Physical Review Research*, **2021**, 3,	3.9	2
78	Some recent developments in auxiliary-field quantum Monte Carlo for real materials. *Journal of Chemical Physics*, **2021**, 154, 024107	3.9	7
77	Ab initio electronic density in solids by many-body plane-wave auxiliary-field quantum Monte Carlo calculations. *Physical Review B*, **2021**, 103,	3.3	2
76	Plaquette versus ordinary d-wave pairing in the t?-Hubbard model on a width-4 cylinder. *Physical Review B*, **2020**, 102,	3.3	12
75	Direct Comparison of Many-Body Methods for Realistic Electronic Hamiltonians. *Physical Review X*, **2020**, 10,	9.1	46
74	Magnetic and charge orders in the ground state of the Emery model: Accurate numerical results. *Physical Review B*, **2020**, 102,	3.3	2
73	Ab Initio Electronic Structure Calculations by Auxiliary-Field Quantum Monte Carlo **2020**, 123-149		2
72	Tuning the quantumness of simple Bose systems: A universal phase diagram. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 27231-27237	11.5	2
71	Absence of Superconductivity in the Pure Two-Dimensional Hubbard Model. *Physical Review X*, **2020**, 10,	9.1	37
70	Ground-State Properties of the Hydrogen Chain: Dimerization, Insulator-to-Metal Transition, and Magnetic Phases. *Physical Review X*, **2020**, 10,	9.1	24
69	Predicting Ligand-Dissociation Energies of 3d Coordination Complexes with Auxiliary-Field Quantum Monte Carlo. *Journal of Chemical Theory and Computation*, **2020**, 16, 3041-3054	6.4	10
68	prediction of annihilators for triplet-triplet annihilation upconversion auxiliary-field quantum Monte Carlo. *Chemical Science*, **2020**, 12, 1068-1079	9.4	1
67	Calculating ground-state properties of correlated fermionic systems with BCS trial wave functions in Slater determinant path-integral approaches. *Physical Review A*, **2019**, 100,	2.6	3
66	Reaching the Continuum Limit in Finite-Temperature Ab□Initio Field-Theory Computations in Many-Fermion Systems. *Physical Review Letters*, **2019**, 123, 136402	7.4	8

65	Efficient Ab Initio Auxiliary-Field Quantum Monte Carlo Calculations in Gaussian Bases via Low-Rank Tensor Decomposition. *Journal of Chemical Theory and Computation*, **2019**, 15, 3510-3521	6.4	26
64	On Achieving High Accuracy in Quantum Chemical Calculations of 3 d Transition Metal-Containing Systems: A Comparison of Auxiliary-Field Quantum Monte Carlo with Coupled Cluster, Density Functional Theory, and Experiment for Diatomic Molecules. *Journal of Chemical Theory and Computation*, **2019**, 15, 2346-2358	6.4	42
63	Metal-insulator transition in the ground state of the three-band Hubbard model at half filling. *Physical Review B*, **2019**, 99,	3.3	9
62	Singlet-Triplet Energy Gaps of Organic Biradicals and Polyacenes with Auxiliary-Field Quantum Monte Carlo. *Journal of Chemical Theory and Computation*, **2019**, 15, 4924-4932	6.4	22
61	Hamiltonian symmetries in auxiliary-field quantum Monte Carlo calculations for electronic structure. *Physical Review B*, **2019**, 100,	3.3	13
60	Local Embedding and Effective Downfolding in the Auxiliary-Field Quantum Monte Carlo Method. *Journal of Chemical Theory and Computation*, **2019**, 15, 3949-3959	6.4	6
59	Charge density waves in a quantum plasma. *Physical Review B*, **2019**, 100,	3.3	1
58	Finite-temperature auxiliary-field quantum Monte Carlo: Self-consistent constraint and systematic approach to low temperatures. *Physical Review B*, **2019**, 99,	3.3	18
57	Accurate computations of Rashba spin-orbit coupling in interacting systems: From the Fermi gas to real materials. *Journal of Physics and Chemistry of Solids*, **2019**, 128, 161-168	3.9	6
56	Communication: Calculation of interatomic forces and optimization of molecular geometry with auxiliary-field quantum Monte Carlo. *Journal of Chemical Physics*, **2018**, 148, 181101	3.9	16
55	Ab Initio Electronic Structure Calculations by Auxiliary-Field Quantum Monte Carlo **2018**, 1-27		3
54	Magnetic orders in the hole-doped three-band Hubbard model: Spin spirals, nematicity, and ferromagnetic domain walls. *Physical Review B*, **2018**, 97,	3.3	6
53	Ab initio computations of molecular systems by the auxiliary-field quantum Monte Carlo method. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2018**, 8, e1364	7.9	63
52	Phaseless Auxiliary-Field Quantum Monte Carlo on Graphical Processing Units. *Journal of Chemical Theory and Computation*, **2018**, 14, 4109-4121	6.4	25
51	Chemical Transformations Approaching Chemical Accuracy via Correlated Sampling in Auxiliary-Field Quantum Monte Carlo. *Journal of Chemical Theory and Computation*, **2017**, 13, 2667-2680	6.4	21
50	Cluster size convergence of the density matrix embedding theory and its dynamical cluster formulation: A study with an auxiliary-field quantum Monte Carlo solver. *Physical Review B*, **2017**, 95,	3.3	28
49	Response Functions for the Two-Dimensional Ultracold Fermi Gas: Dynamical BCS Theory and Beyond. *Journal of Low Temperature Physics*, **2017**, 189, 312-327	1.3	4
48	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,	9.1	121

47	Computation of Ground-State Properties in Molecular Systems: Back-Propagation with Auxiliary-Field Quantum Monte Carlo. *Journal of Chemical Theory and Computation*, **2017**, 13, 5367-5378	6.4	32
46	Many-body computations by stochastic sampling in Hartree-Fock-Bogoliubov space. *Physical Review B*, **2017**, 95,	3.3	13
45	Stripe order in the underdoped region of the two-dimensional Hubbard model. *Science*, **2017**, 358, 1155-1160	33.9	215
44	High-field magnetization and magnetic phase diagram of Cu2V2O7. *Physical Review B*, **2017**, 95,	3.3	15
43	Ultracold Atoms in a Square Lattice with Spin-Orbit Coupling: Charge Order, Superfluidity, and Topological Signatures. *Physical Review Letters*, **2017**, 119, 265301	7.4	13
42	Computation of dynamical correlation functions for many-fermion systems with auxiliary-field quantum Monte Carlo. *Physical Review B*, **2016**, 94,	3.3	31
41	Infinite variance in fermion quantum Monte Carlo calculations. *Physical Review E*, **2016**, 93, 033303	2.4	30
40	Majorana Positivity and the Fermion Sign Problem of Quantum Monte Carlo Simulations. *Physical Review Letters*, **2016**, 116, 250601	7.4	49
39	Rashba Spin-Orbit Coupling, Strong Interactions, and the BCS-BEC Crossover in the Ground State of the Two-Dimensional Fermi Gas. *Physical Review Letters*, **2016**, 117, 040401	7.4	13
38	Benchmark study of the two-dimensional Hubbard model with auxiliary-field quantum Monte Carlo method. *Physical Review B*, **2016**, 94,	3.3	38
37	Coupling quantum Monte Carlo and independent-particle calculations: Self-consistent constraint for the sign problem based on the density or the density matrix. *Physical Review B*, **2016**, 94,	3.3	24
36	Auxiliary-field quantum Monte Carlo calculations of the molybdenum dimer. *Journal of Chemical Physics*, **2016**, 144, 244306	3.9	9
35	An auxiliary-field quantum Monte Carlo study of the chromium dimer. *Journal of Chemical Physics*, **2015**, 142, 064302	3.9	44
34	Ground-state properties of strongly interacting Fermi gases in two dimensions. *Physical Review A*, **2015**, 92,	2.6	58
33	Quantum Monte Carlo Calculations in Solids with Downfolded Hamiltonians. *Physical Review Letters* , **2015**, 114, 226401	7.4	40
32	Solutions of the Two-Dimensional Hubbard Model: Benchmarks and Results from a Wide Range of Numerical Algorithms. *Physical Review X*, **2015**, 5,	9.1	269
31	Stability, energetics, and magnetic states of cobalt adatoms on graphene. *Physical Review Letters*, **2014**, 113, 175502	7.4	38
30	Symmetry-projected wave functions in quantum Monte Carlo calculations. *Physical Review B*, **2014**, 89,	3.3	36

29	Phases of attractive spin-imbalanced fermions in square lattices. *Physical Review A*, **2013**, 88,	2.6	11
28	Frozen-Orbital and Downfolding Calculations with Auxiliary-Field Quantum Monte Carlo. *Journal of Chemical Theory and Computation*, **2013**, 9, 4825-33	6.4	26
27	Excited state calculations in solids by auxiliary-field quantum Monte Carlo. *New Journal of Physics*, **2013**, 15, 093017	2.9	33
26	Symmetry in auxiliary-field quantum Monte Carlo calculations. *Physical Review B*, **2013**, 88,	3.3	56
25	Finite-temperature auxiliary-field quantum Monte Carlo technique for Bose-Fermi mixtures. *Physical Review A*, **2012**, 86,	2.6	23
24	Spin- and charge-density waves in the Hartree-Fock ground state of the two-dimensional Hubbard model. *Journal of Physics Condensed Matter*, **2011**, 23, 505601	1.8	17
23	Auxiliary-field quantum Monte Carlo method for strongly paired fermions. *Physical Review A*, **2011**, 84,	2.6	98
22	Assessing weak hydrogen binding on Ca+ centers: an accurate many-body study with large basis sets. *Journal of Chemical Physics*, **2011**, 135, 164105	3.9	41
21	Spin and charge order in the doped hubbard model: long-wavelength collective modes. *Physical Review Letters*, **2010**, 104, 116402	7.4	64
20	Itinerant ferromagnetism in a Fermi gas with contact interaction: Magnetic properties in a dilute Hubbard model. *Physical Review A*, **2010**, 82,	2.6	18
19	Pressure-induced diamond to β-tin transition in bulk silicon: A quantum Monte Carlo study. *Physical Review B*, **2009**, 80,	3.3	50
18	Excited state calculations using phaseless auxiliary-field quantum Monte Carlo: Potential energy curves of low-lying C(2) singlet states. *Journal of Chemical Physics*, **2009**, 130, 094107	3.9	54
17	Eliminating spin contamination in auxiliary-field quantum Monte Carlo: realistic potential energy curve of F(2). *Journal of Chemical Physics*, **2008**, 128, 114309	3.9	47
16	Finite-size correction in many-body electronic structure calculations. *Physical Review Letters*, **2008**, 100, 126404	7.4	93
15	Hartree-Fock ground state of the three-dimensional electron gas. *Physical Review Letters*, **2008**, 100, 236404	7.4	31
14	Spatially inhomogeneous phase in the two-dimensional repulsive Hubbard model. *Physical Review B* , **2008**, 78,	3.3	62
13	Bond breaking with auxiliary-field quantum Monte Carlo. *Journal of Chemical Physics*, **2007**, 127, 144101	3.9	40
12	Phaseless auxiliary-field quantum Monte Carlo calculations with plane waves and pseudopotentials: Applications to atoms and molecules. *Physical Review B*, **2007**, 75,	3.3	55

11	Auxiliary-field quantum Monte Carlo calculations of molecular systems with a Gaussian basis. *Journal of Chemical Physics*, **2006**, 124, 224101	3.9	69
10	Correlation effects in the ground state of trapped atomic Bose gases. *Physical Review A*, **2005**, 72,	2.6	27
9	Quantum Monte Carlo method for the ground state of many-boson systems. *Physical Review E*, **2004**, 70, 056702	2.4	54
8	Quantum Monte Carlo method using phase-free random walks with slater determinants. *Physical Review Letters*, **2003**, 90, 136401	7.4	213
7	Constrained-path quantum Monte Carlo simulations of the zero-temperature disordered two-dimensional Hubbard model. *Physical Review B*, **2001**, 64,	3.3	7
6	Finite-Temperature Monte Carlo Calculations for Systems with Fermions. *Physical Review Letters*, **1999**, 83, 2777-2780	7.4	38
5	Issues and observations on applications of the constrained-path Monte Carlo method to many-fermion systems. *Physical Review B*, **1999**, 59, 12788-12798	3.3	40
4	Bunching Transitions on Vicinal Surfaces and Quantum n-mers. *Physical Review Letters*, **1998**, 81, 3475-3478	7.4	31
3	Constrained path Monte Carlo method for fermion ground states. *Physical Review B*, **1997**, 55, 7464-7477	3.3	251
2	Pairing Correlations in the Two-Dimensional Hubbard Model. *Physical Review Letters*, **1997**, 78, 4486-4489	7.4	138
1	Constrained path quantum Monte Carlo method for fermion ground states. *Physical Review Letters*, **1995**, 74, 3652-3655	7.4	143