Garnet Chan

List of Publications by Year
in descending order

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126 papers	12,583 citations	25034 57 h-index	24258 110 g-index
132 all docs	132 docs citations	132 times ranked	5428 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	The Density Matrix Renormalization Group in Quantum Chemistry. Annual Review of Physical Chemistry, 2011, 62, 465-481.	10.8	572
3	Highly correlated calculations with a polynomial cost algorithm: A study of the density matrix renormalization group. Journal of Chemical Physics, 2002, 116, 4462-4476.	3.0	459
4	The radical character of the acenes: A density matrix renormalization group study. Journal of Chemical Physics, 2007, 127, 134309.	3.0	421
5	Solutions of the Two-Dimensional Hubbard Model: Benchmarks and Results from a Wide Range of Numerical Algorithms. Physical Review X, 2015, 5, .	8.9	398
6	Recent developments in the P<scp>y</scp>SCF program package. Journal of Chemical Physics, 2020, 153, 024109.	3.0	388
7	Stripe order in the underdoped region of the two-dimensional Hubbard model. Science, 2017, 358, 1155-1160.	12.6	368
8	Density Matrix Embedding: A Simple Alternative to Dynamical Mean-Field Theory. Physical Review Letters, 2012, 109, 186404.	7.8	353
9	Determining eigenstates and thermal states on a quantum computer using quantum imaginary time evolution. Nature Physics, 2020, 16, 205-210.	16.7	317
10	Quantum Algorithms for Quantum Chemistry and Quantum Materials Science. Chemical Reviews, 2020, 120, 12685-12717.	47.7	311
11	Orbital optimization in the density matrix renormalization group, with applications to polyenes and Î²-carotene. Journal of Chemical Physics, 2008, 128, 144117.	3.0	288
12	The ab-initio density matrix renormalization group in practice. Journal of Chemical Physics, 2015, 142, 034102.	3.0	266
13	Quantum Simulation of Electronic Structure with Linear Depth and Connectivity. Physical Review Letters, 2018, 120, 110501.	7.8	243
14	Density Matrix Embedding: A Strong-Coupling Quantum Embedding Theory. Journal of Chemical Theory and Computation, 2013, 9, 1428-1432.	5.3	238
15	Ab initio determination of the crystalline benzene lattice energy to sub-kilojoule/mole accuracy. Science, 2014, 345, 640-643.	12.6	230
16	Spin-adapted density matrix renormalization group algorithms for quantum chemistry. Journal of Chemical Physics, 2012, 136, 124121.	3.0	229
17	Low-energy spectrum of ironâ€“sulfur clusters directly from many-particle quantum mechanics. Nature Chemistry, 2014, 6, 927-933.	13.6	227
18	Entangled quantum electronic wavefunctions of the Mn4CaO5 cluster in photosystem II. Nature Chemistry, 2013, 5, 660-666.	13.6	215

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19	Canonical transformation theory for multireference problems. Journal of Chemical Physics, 2006, 124, 194106.	3.0	204
20	Quantum Embedding Theories. Accounts of Chemical Research, 2016, 49, 2705-2712.	15.6	200
21	Low-Depth Quantum Simulation of Materials. Physical Review X, 2018, 8, .	8.9	187
22	An algorithm for large scale density matrix renormalization group calculations. Journal of Chemical Physics, 2004, 120, 3172-3178.	3.0	174
23	Multireference correlation in long molecules with the quadratic scaling density matrix renormalization group. Journal of Chemical Physics, 2006, 125, 144101.	3.0	174
24	State-of-the-art density matrix renormalization group and coupled cluster theory studies of the nitrogen binding curve. Journal of Chemical Physics, 2004, 121, 6110-6116.	3.0	172
25	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
26	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
27	The orbital-specific-virtual local coupled cluster singles and doubles method. Journal of Chemical Physics, 2012, 136, 144105.	3.0	163
28	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
29	Ground-state phase diagram of the square lattice Hubbard model from density matrix embedding theory. Physical Review B, 2016, 93, .	3.2	138
30	Exact parameterization of fermionic wave functions via unitary coupled cluster theory. Journal of Chemical Physics, 2019, 151, 244112.	3.0	124
31	Canonical transformation theory from extended normal ordering. Journal of Chemical Physics, 2007, 127, 104107.	3.0	122
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	Automated Construction of Molecular Active Spaces from Atomic Valence Orbitals. Journal of Chemical Theory and Computation, 2017, 13, 4063-4078.	5.3	119
34	Efficient tree tensor network states (TTNS) for quantum chemistry: Generalizations of the density matrix renormalization group algorithm. Journal of Chemical Physics, 2013, 138, 134113.	3.0	110
35	Exact solution (within a triple-zeta, double polarization basis set) of the electronic SchrÃ¶dinger equation for water. Journal of Chemical Physics, 2003, 118, 8551-8554.	3.0	109
36	Communication: A flexible multi-reference perturbation theory by minimizing the Hylleraas functional with matrix product states. Journal of Chemical Physics, 2014, 141, 111101.	3.0	90

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37	The Ground State Electronic Energy of Benzene. Journal of Physical Chemistry Letters, 2020, 11, 8922-8929.	4.6	90
38	A review of canonical transformation theory. International Reviews in Physical Chemistry, 2010, 29, 231-271.	2.3	86
39	Accelerating convergence in iterative solution for largeâ€scale complete active space selfâ€consistentâ€field calculations. International Journal of Quantum Chemistry, 2009, 109, 2178-2190.	2.0	84
40	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
41	Time-Dependent Density Matrix Renormalization Group Algorithms for Nearly Exact Absorption and Fluorescence Spectra of Molecular Aggregates at Both Zero and Finite Temperature. Journal of Chemical Theory and Computation, 2018, 14, 5027-5039.	5.3	83
42	Excited States of Butadiene to Chemical Accuracy: Reconciling Theory and Experiment. Journal of Chemical Theory and Computation, 2012, 8, 4013-4018.	5.3	82
43	Quadratic canonical transformation theory and higher order density matrices. Journal of Chemical Physics, 2009, 130, 124102.	3.0	81
44	Tailored coupled cluster singles and doubles method applied to calculations on molecular structure and harmonic vibrational frequencies of ozone. Journal of Chemical Physics, 2006, 124, 114311.	3.0	80
45	Spectroscopic accuracy directly from quantum chemistry: Application to ground and excited states of beryllium dimer. Journal of Chemical Physics, 2014, 140, 104112.	3.0	75
46	A fresh look at ensembles: Derivative discontinuities in density functional theory. Journal of Chemical Physics, 1999, 110, 4710-4723.	3.0	73
47	Chapter 7 The Density Matrix Renormalization Group in Quantum Chemistry. Annual Reports in Computational Chemistry, 2009, 5, 149-162.	1.7	72
48	A study of cumulant approximations to n-electron valence multireference perturbation theory. Journal of Chemical Physics, 2009, 130, 194107.	3.0	70
49	Excited-State Geometry Optimization with the Density Matrix Renormalization Group, as Applied to Polyenes. Journal of Chemical Theory and Computation, 2015, 11, 3000-3009.	5.3	70
50	Spectral functions of the uniform electron gas via coupled-cluster theory and comparison to the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m related approximations. Physical Review B, 2016, 93, .	3.2	70
51	Quantum Computation of Finite-Temperature Static and Dynamical Properties of Spin Systems Using Quantum Imaginary Time Evolution. PRX Quantum, 2021, 2, .	9.2	68
52	Optimized Lieb-Oxford bound for the exchange-correlation energy. Physical Review A, 1999, 59, 3075-3077.	2.5	67
53	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
54	Gaussian and plane-wave mixed density fitting for periodic systems. Journal of Chemical Physics, 2017, 147, 164119.	3.0	66

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55	Time-Dependent Density Functional Theory of Classical Fluids. Physical Review Letters, 2005, 94, 183001.	7.8	64
56	Efficient Implementation of Ab Initio Quantumâ€Embedding in Periodic Systems: Density Matrixâ€Embedding Theory. Journal of Chemical Theory and Computation, 2020, 16, 119-129.	5.3	64
57	Thomasâ€“Fermiâ€“Diracâ€“von Weizsaˆcker models in finite systems. Journal of Chemical Physics, 2001, 114, 631.	3.0	59
58	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
59	Density-matrix renormalization-group algorithms with nonorthogonal orbitals and non-Hermitian operators, and applications to polyenes. Journal of Chemical Physics, 2005, 122, 204101.	3.0	56
60	From plane waves to local Gaussians for the simulation of correlated periodic systems. Journal of Chemical Physics, 2016, 145, 084111.	3.0	56
61	Analytic response theory for the density matrix renormalization group. Journal of Chemical Physics, 2009, 130, 184111.	3.0	55
62	Low rank representations for quantum simulation of electronic structure. Npj Quantum Information, 2021, 7, .	6.7	54
63	A time-dependent formulation of multi-reference perturbation theory. Journal of Chemical Physics, 2016, 144, 064102.	3.0	53
64	Exact Fluctuations of Nonequilibrium Steady States from Approximate Auxiliary Dynamics. Physical Review Letters, 2018, 120, 210602.	7.8	50
65	Low communication high performance ab initio density matrix renormalization group algorithms. Journal of Chemical Physics, 2021, 154, 224116.	3.0	49
66	Kinetic-energy systems, density scaling, and homogeneity relations in density-functional theory. Physical Review A, 1999, 59, 2670-2679.	2.5	48
67	Communication: Excited states, dynamic correlation functions and spectral properties from full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2012, 137, 191102.	3.0	47
68	Intermediate and spin-liquid phase of the half-filled honeycomb Hubbard model. Physical Review B, 2014, 89, .	3.2	47
69	Time-dependent N-electron valence perturbation theory with matrix product state reference wavefunctions for large active spaces and basis sets: Applications to the chromium dimer and all-trans polyenes. Journal of Chemical Physics, 2017, 146, 244102.	3.0	47
70	A Time-Dependent Formulation of Coupled-Cluster Theory for Many-Fermion Systems at Finite Temperature. Journal of Chemical Theory and Computation, 2018, 14, 5690-5700.	5.3	47
71	Linear response theory for the density matrix renormalization group: Efficient algorithms for strongly correlated excited states. Journal of Chemical Physics, 2014, 140, 024108.	3.0	46
72	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

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73	An extensive study of gradient approximations to the exchange-correlation and kinetic energy functionals. Journal of Chemical Physics, 2000, 112, 5639-5653.	3.0	43
74	Ground-State Properties of the Hydrogen Chain: Dimerization, Insulator-to-Metal Transition, and Magnetic Phases. Physical Review X, 2020, 10, .	8.9	42
75	Importance sampling large deviations in nonequilibrium steady states. I. Journal of Chemical Physics, 2018, 148, 124120.	3.0	40
76	Efficient Formulation of Ab Initio Quantum Embedding in Periodic Systems: Dynamical Mean-Field Theory. Journal of Chemical Theory and Computation, 2020, 16, 141-153.	5.3	40
77	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.	5.3	39
78	Thouless theorem for matrix product states and subsequent post density matrix renormalization group methods. Physical Review B, 2013, 88, .	3.2	38
79	Exact and Optimal Quantum Mechanics/Molecular Mechanics Boundaries. Journal of Chemical Theory and Computation, 2014, 10, 3784-3790.	5.3	37
80	Coupled-cluster impurity solvers for dynamical mean-field theory. Physical Review B, 2019, 100, .	3.2	37
81	Density matrix renormalisation group Lagrangians. Physical Chemistry Chemical Physics, 2008, 10, 3454.	2.8	34
82	Striped Spin Liquid Crystal Ground State Instability of Kagome Antiferromagnets. Physical Review Letters, 2013, 111, 187205.	7.8	34
83	Spin-Projected Matrix Product States: Versatile Tool for Strongly Correlated Systems. Journal of Chemical Theory and Computation, 2017, 13, 2681-2695.	5.3	34
84	A state interaction spin-orbit coupling density matrix renormalization group method. Journal of Chemical Physics, 2016, 144, 234301.	3.0	33
85	AbÂInitio Full Cell <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi><mml:mo>+</mml:mo><mml:mi>DMFT</mml:mi></mml:mrow></mml:math> for Correlated Materials. Physical Review X, 2021, 11, .	8.9	33
86	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, .	3.2	32
87	A Perturbative Density Matrix Renormalization Group Algorithm for Large Active Spaces. Journal of Chemical Theory and Computation, 2018, 14, 4063-4071.	5.3	32
88	All-Electron Gaussian-Based G₀W₀ for Valence and Core Excitation Energies of Periodic Systems. Journal of Chemical Theory and Computation, 2021, 17, 727-741.	5.3	32
89	Dynamical phase behavior of the single- and multi-lane asymmetric simple exclusion process via matrix product states. Physical Review E, 2019, 100, 022101.	2.1	28
90	A real-time extension of density matrix embedding theory for non-equilibrium electron dynamics. Journal of Chemical Physics, 2018, 148, 054108.	3.0	27

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91	Electronic structure of bulk manganese oxide and nickel oxide from coupled cluster theory. Physical Review B, 2020, 101, .	3.2	27
92	Conversion of projected entangled pair states into a canonical form. Physical Review B, 2019, 100, .	3.2	26
93	Variational Power of Quantum Circuit Tensor Networks. Physical Review X, 2022, 12, .	8.9	23
94	Lowering of the complexity of quantum chemistry methods by choice of representation. Journal of Chemical Physics, 2018, 148, 044106.	3.0	22
95	Projected density matrix embedding theory with applications to the two-dimensional Hubbard model. Journal of Chemical Physics, 2019, 151, .	3.0	22
96	Ground-state phase diagram of the three-band Hubbard model from density matrix embedding theory. Physical Review Research, 2020, 2, .	3.6	22
97	Dynamical Phase Transitions in a 2D Classical Nonequilibrium Model via 2D Tensor Networks. Physical Review Letters, 2020, 125, 140601.	7.8	21
98	Electron paramagnetic resonance g-tensors from state interaction spin-orbit coupling density matrix renormalization group. Journal of Chemical Physics, 2018, 148, 184103.	3.0	20
99	Finite-temperature density matrix embedding theory. Physical Review B, 2020, 101, .	3.2	20
100	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
101	Hamiltonian symmetries in auxiliary-field quantum Monte Carlo calculations for electronic structure. Physical Review B, 2019, 100, .	3.2	19
102	Externally Corrected CCSD with Renormalized Perturbative Triples (R-ecCCSD(T)) and the Density Matrix Renormalization Group and Selected Configuration Interaction External Sources. Journal of Chemical Theory and Computation, 2021, 17, 3414-3425.	5.3	18
103	Constructing tensor network influence functionals for general quantum dynamics. Journal of Chemical Physics, 2021, 155, 044104.	3.0	18
104	Theoretical prediction of magnetic exchange coupling constants from broken-symmetry coupled cluster calculations. Journal of Chemical Physics, 2020, 152, 234115.	3.0	17
105	A coupled cluster framework for electrons and phonons. Journal of Chemical Physics, 2020, 153, 224112.	3.0	17
106	Matrix Product States with Large Sites. Journal of Chemical Theory and Computation, 2022, 18, 749-762.	5.3	17
107	Projector quantum Monte Carlo with matrix product states. Physical Review B, 2014, 90, .	3.2	16
108	Finite-temperature coupled cluster: Efficient implementation and application to prototypical systems. Journal of Chemical Physics, 2020, 152, 224104.	3.0	16

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109	Correlator product state study of molecular magnetism in the giant Keplerate Mo<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>72</mml:mn></mml:msub></mml:math>Fe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>30</mml:mn></mml:msub></mml:math>. Physical Review B, 2012, 86, .	3.2	15
110	Time-Dependent Coupled Cluster Theory on the Keldysh Contour for Nonequilibrium Systems. Journal of Chemical Theory and Computation, 2019, 15, 6137-6153.	5.3	15
111	Finite and infinite matrix product states for Gutzwiller projected mean-field wave functions. Physical Review B, 2021, 103, .	3.2	13
112	Correct Quantum Chemistry in a Minimal Basis from Effective Hamiltonians. Journal of Chemical Theory and Computation, 2016, 12, 512-522.	5.3	12
113	Efficient representation of long-range interactions in tensor network algorithms. Physical Review B, 2018, 98, .	3.2	11
114	Constructing auxiliary dynamics for nonequilibrium stationary states by variance minimization. Journal of Chemical Physics, 2020, 152, 104107.	3.0	10
115	A transformed framework for dynamic correlation in multireference problems. Journal of Chemical Physics, 2015, 142, 124107.	3.0	9
116	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
117	Exploring the Magnetic Properties of the Largest Single-Molecule Magnets. Journal of Physical Chemistry Letters, 2020, 11, 3789-3795.	4.6	9
118	The Fermionic Quantum Emulator. Quantum - the Open Journal for Quantum Science, 0, 5, 568.	0.0	9
119	Stimulated X-ray Raman and Absorption Spectroscopy of Ironâ€“Sulfur Dimers. Journal of Physical Chemistry Letters, 2019, 10, 6664-6671.	4.6	8
120	Pure State v-Representability of Density Matrix Embedding Theory. Journal of Chemical Theory and Computation, 2022, 18, 851-864.	5.3	8
121	Minimal Matrix Product States and Generalizations of Mean-Field and Geminal Wave Functions. Journal of Chemical Theory and Computation, 2020, 16, 5057-5066.	5.3	7
122	Conservation laws in coupled cluster dynamics at finite temperature. Journal of Chemical Physics, 2021, 155, 044103.	3.0	7
123	Hilbert space renormalization for the many-electron problem. Journal of Chemical Physics, 2016, 144, 084103.	3.0	5
124	The Fate of Atomic Spin in Atomic Scattering off Surfaces. Journal of Physical Chemistry Letters, 2018, 9, 2863-2868.	4.6	4
125	Using Hyperoptimized Tensor Networks and First-Principles Electronic Structure to Simulate the Experimental Properties of the Giant {Mn₈₄} Torus. Journal of Physical Chemistry Letters, 2022, 13, 2365-2370.	4.6	3
126	Numerical continuum tensor networks in two dimensions. Physical Review Research, 2021, 3, .	3.6	1