

Garnet Chan

List of Publications by Year in descending order

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126
papers

12,583
citations

25034

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110
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all docs

132
docs citations

132
times ranked

5428
citing authors

#	ARTICLE	IF	CITATIONS
1	Pure State $\langle i v \langle i $ -Representability of Density Matrix Embedding Theory. Journal of Chemical Theory and Computation, 2022, 18, 851-864.	5.3	8
2	Matrix Product States with Large Sites. Journal of Chemical Theory and Computation, 2022, 18, 749-762.	5.3	17
3	Variational Power of Quantum Circuit Tensor Networks. Physical Review X, 2022, 12, .	8.9	23
4	Using Hyperoptimized Tensor Networks and First-Principles Electronic Structure to Simulate the Experimental Properties of the Giant $\{Mn_{84}\}$ Torus. Journal of Physical Chemistry Letters, 2022, 13, 2365-2370.	4.6	3
5	All-Electron Gaussian-Based $\langle i G \langle i \langle sub \rangle 0 \langle /sub \rangle \langle i W \langle i \langle sub \rangle 0 \langle /sub \rangle$ for Valence and Core Excitation Energies of Periodic Systems. Journal of Chemical Theory and Computation, 2021, 17, 727-741.	5.3	32
6	Quantum Computation of Finite-Temperature Static and Dynamical Properties of Spin Systems Using Quantum Imaginary Time Evolution. PRX Quantum, 2021, 2, .	9.2	68
7	Finite and infinite matrix product states for Gutzwiller projected mean-field wave functions. Physical Review B, 2021, 103, .	3.2	13
8	Numerical continuum tensor networks in two dimensions. Physical Review Research, 2021, 3, .	3.6	1
9	$\langle i \text{Ab Initio} \langle /i \rangle$ Full Cell $\langle mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" \rangle \langle mml:mrow \rangle \langle mml:mi \rangle G \langle /mml:mi \rangle \langle mml:mi \rangle W \langle /mml:mi \rangle \langle mml:mo \rangle + \langle /mml:mo \rangle \langle mml:mi \rangle DMFT \langle /mml:mi \rangle \langle mml:mo \rangle \langle mml:mi \rangle \langle /mml:mi \rangle$ for Correlated Materials. Physical Review X, 2021, 11, .	3.3	13
10	Low rank representations for quantum simulation of electronic structure. Npj Quantum Information, 2021, 7, .	6.7	54
11	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
12	Low communication high performance $\langle i \rangle \text{ab initio} \langle /i \rangle$ density matrix renormalization group algorithms. Journal of Chemical Physics, 2021, 154, 224116.	3.0	49
13	Conservation laws in coupled cluster dynamics at finite temperature. Journal of Chemical Physics, 2021, 155, 044103.	3.0	7
14	Constructing tensor network influence functionals for general quantum dynamics. Journal of Chemical Physics, 2021, 155, 044104.	3.0	18
15	Determining eigenstates and thermal states on a quantum computer using quantum imaginary time evolution. Nature Physics, 2020, 16, 205-210.	16.7	317
16	Efficient Implementation of Ab Initio Quantum Embedding in Periodic Systems: Density Matrix Embedding Theory. Journal of Chemical Theory and Computation, 2020, 16, 119-129.	5.3	64
17	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
18	Dynamical Phase Transitions in a 2D Classical Nonequilibrium Model via 2D Tensor Networks. Physical Review Letters, 2020, 125, 140601.	7.8	21

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19	Quantum Algorithms for Quantum Chemistry and Quantum Materials Science. <i>Chemical Reviews</i> , 2020, 120, 12685-12717.	47.7	311
20	The Ground State Electronic Energy of Benzene. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 8922-8929.	4.6	90
21	Recent developments in the PySCF program package. <i>Journal of Chemical Physics</i> , 2020, 153, 024109.	3.0	388
22	Ground-State Properties of the Hydrogen Chain: Dimerization, Insulator-to-Metal Transition, and Magnetic Phases. <i>Physical Review X</i> , 2020, 10, .	8.9	42
23	Minimal Matrix Product States and Generalizations of Mean-Field and Geminal Wave Functions. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 5057-5066.	5.3	7
24	Constructing auxiliary dynamics for nonequilibrium stationary states by variance minimization. <i>Journal of Chemical Physics</i> , 2020, 152, 104107.	3.0	10
25	Finite-temperature coupled cluster: Efficient implementation and application to prototypical systems. <i>Journal of Chemical Physics</i> , 2020, 152, 224104.	3.0	16
26	Theoretical prediction of magnetic exchange coupling constants from broken-symmetry coupled cluster calculations. <i>Journal of Chemical Physics</i> , 2020, 152, 234115.	3.0	17
27	Finite-temperature density matrix embedding theory. <i>Physical Review B</i> , 2020, 101, .	3.2	20
28	Electronic structure of bulk manganese oxide and nickel oxide from coupled cluster theory. <i>Physical Review B</i> , 2020, 101, .	3.2	27
29	Exploring the Magnetic Properties of the Largest Single-Molecule Magnets. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 3789-3795.	4.6	9
30	A coupled cluster framework for electrons and phonons. <i>Journal of Chemical Physics</i> , 2020, 153, 224112.	3.0	17
31	Ground-state phase diagram of the three-band Hubbard model from density matrix embedding theory. <i>Physical Review Research</i> , 2020, 2, .	3.6	22
32	Conversion of projected entangled pair states into a canonical form. <i>Physical Review B</i> , 2019, 100, .	3.2	26
33	Dynamical phase behavior of the single- and multi-lane asymmetric simple exclusion process via matrix product states. <i>Physical Review E</i> , 2019, 100, 022101.	2.1	28
34	Hamiltonian symmetries in auxiliary-field quantum Monte Carlo calculations for electronic structure. <i>Physical Review B</i> , 2019, 100, .	3.2	19
35	Generalization of the exponential basis for tensor network representations of long-range interactions in two and three dimensions. <i>Physical Review B</i> , 2019, 100, .	3.2	9
36	Time-Dependent Coupled Cluster Theory on the Keldysh Contour for Nonequilibrium Systems. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6137-6153.	5.3	15

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37	Projected density matrix embedding theory with applications to the two-dimensional Hubbard model. <i>Journal of Chemical Physics</i> , 2019, 151, .	3.0	22
38	Coupled-cluster impurity solvers for dynamical mean-field theory. <i>Physical Review B</i> , 2019, 100, .	3.2	37
39	Stimulated X-ray Raman and Absorption Spectroscopy of Ironâ€Sulfur Dimers. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 6664-6671.	4.6	8
40	Electronic landscape of the P-cluster of nitrogenase as revealed through many-electron quantum wavefunction simulations. <i>Nature Chemistry</i> , 2019, 11, 1026-1033.	13.6	67
41	Efficient Ab Initio Auxiliary-Field Quantum Monte Carlo Calculations in Gaussian Bases via Low-Rank Tensor Decomposition. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 3510-3521.	5.3	39
42	Exact parameterization of fermionic wave functions via unitary coupled cluster theory. <i>Journal of Chemical Physics</i> , 2019, 151, 244112.	3.0	124
43	The electronic complexity of the ground-state of the FeMo cofactor of nitrogenase as relevant to quantum simulations. <i>Journal of Chemical Physics</i> , 2019, 150, 024302.	3.0	59
44	Lowering of the complexity of quantum chemistry methods by choice of representation. <i>Journal of Chemical Physics</i> , 2018, 148, 044106.	3.0	22
45	Importance sampling large deviations in nonequilibrium steady states. I. <i>Journal of Chemical Physics</i> , 2018, 148, 124120.	3.0	40
46	A real-time extension of density matrix embedding theory for non-equilibrium electron dynamics. <i>Journal of Chemical Physics</i> , 2018, 148, 054108.	3.0	27
47	Low-Depth Quantum Simulation of Materials. <i>Physical Review X</i> , 2018, 8, .	8.9	187
48	Quantum Simulation of Electronic Structure with Linear Depth and Connectivity. <i>Physical Review Letters</i> , 2018, 120, 110501.	7.8	243
49	P<sc>y</sc>SCF: the Pythonâ€based simulations of chemistry framework. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2018, 8, e1340.	14.6	894
50	Efficient representation of long-range interactions in tensor network algorithms. <i>Physical Review B</i> , 2018, 98, .	3.2	11
51	A Time-Dependent Formulation of Coupled-Cluster Theory for Many-Fermion Systems at Finite Temperature. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 5690-5700.	5.3	47
52	The Fate of Atomic Spin in Atomic Scattering off Surfaces. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 2863-2868.	4.6	4
53	Exact Fluctuations of Nonequilibrium Steady States from Approximate Auxiliary Dynamics. <i>Physical Review Letters</i> , 2018, 120, 210602.	7.8	50
54	Electron paramagnetic resonance g-tensors from state interaction spin-orbit coupling density matrix renormalization group. <i>Journal of Chemical Physics</i> , 2018, 148, 184103.	3.0	20

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55	A Perturbative Density Matrix Renormalization Group Algorithm for Large Active Spaces. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4063-4071.	5.3	32
56	Communication: An efficient stochastic algorithm for the perturbative density matrix renormalization group in large active spaces. <i>Journal of Chemical Physics</i> , 2018, 148, 221104.	3.0	19
57	Time-Dependent Density Matrix Renormalization Group Algorithms for Nearly Exact Absorption and Fluorescence Spectra of Molecular Aggregates at Both Zero and Finite Temperature. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 5027-5039.	5.3	83
58	Gaussian-Based Coupled-Cluster Theory for the Ground-State and Band Structure of Solids. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1209-1218.	5.3	171
59	Spin-Projected Matrix Product States: Versatile Tool for Strongly Correlated Systems. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2681-2695.	5.3	34
60	Cluster size convergence of the density matrix embedding theory and its dynamical cluster formulation: A study with an auxiliary-field quantum Monte Carlo solver. <i>Physical Review B</i> , 2017, 95, .	3.2	32
61	A general second order complete active space self-consistent-field solver for large-scale systems. <i>Chemical Physics Letters</i> , 2017, 683, 291-299.	2.6	84
62	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. <i>Physical Review X</i> , 2017, 7, .	8.9	171
63	Time-Step Targeting Time-Dependent and Dynamical Density Matrix Renormalization Group Algorithms with ab Initio Hamiltonians. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5560-5571.	5.3	45
64	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. <i>Journal of Chemical Physics</i> , 2017, 146, 244102.	3.0	47
65	Automated Construction of Molecular Active Spaces from Atomic Valence Orbitals. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4063-4078.	5.3	119
66	Stripe order in the underdoped region of the two-dimensional Hubbard model. <i>Science</i> , 2017, 358, 1155-1160.	12.6	368
67	Gaussian and plane-wave mixed density fitting for periodic systems. <i>Journal of Chemical Physics</i> , 2017, 147, 164119.	3.0	66
68	From plane waves to local Gaussians for the simulation of correlated periodic systems. <i>Journal of Chemical Physics</i> , 2016, 145, 084111.	3.0	56
69	Matrix product operators, matrix product states, and ab initio density matrix renormalization group algorithms. <i>Journal of Chemical Physics</i> , 2016, 145, 014102.	3.0	121
70	A state interaction spin-orbit coupling density matrix renormalization group method. <i>Journal of Chemical Physics</i> , 2016, 144, 234301.	3.0	33
71	A time-dependent formulation of multi-reference perturbation theory. <i>Journal of Chemical Physics</i> , 2016, 144, 064102.	3.0	53
72	Hilbert space renormalization for the many-electron problem. <i>Journal of Chemical Physics</i> , 2016, 144, 084103.	3.0	5

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73	Ground-state phase diagram of the square lattice Hubbard model from density matrix embedding theory. <i>Physical Review B</i> , 2016, 93, .	3.2	138
74	Spectral functions of the uniform electron gas via coupled-cluster theory and comparison to the related approximations. <i>Physical Review B</i> , 2016, 93, .	3.2	70
75	Quantum Embedding Theories. <i>Accounts of Chemical Research</i> , 2016, 49, 2705-2712.	15.6	200
76	<i>N</i> -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(<i>p</i> -Phenylenevinylene). <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1583-1591.	5.3	145
77	Correct Quantum Chemistry in a Minimal Basis from Effective Hamiltonians. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 512-522.	5.3	12
78	Excited-State Geometry Optimization with the Density Matrix Renormalization Group, as Applied to Polyenes. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3000-3009.	5.3	70
79	A transformed framework for dynamic correlation in multireference problems. <i>Journal of Chemical Physics</i> , 2015, 142, 124107.	3.0	9
80	Solutions of the Two-Dimensional Hubbard Model: Benchmarks and Results from a Wide Range of Numerical Algorithms. <i>Physical Review X</i> , 2015, 5, .	8.9	398
81	The <i>ab-initio</i> density matrix renormalization group in practice. <i>Journal of Chemical Physics</i> , 2015, 142, 034102.	3.0	266
82	Communication: A flexible multi-reference perturbation theory by minimizing the Hylleraas functional with matrix product states. <i>Journal of Chemical Physics</i> , 2014, 141, 111101.	3.0	90
83	Linear response theory for the density matrix renormalization group: Efficient algorithms for strongly correlated excited states. <i>Journal of Chemical Physics</i> , 2014, 140, 024108.	3.0	46
84	Projector quantum Monte Carlo with matrix product states. <i>Physical Review B</i> , 2014, 90, .	3.2	16
85	Intermediate and spin-liquid phase of the half-filled honeycomb Hubbard model. <i>Physical Review B</i> , 2014, 89, .	3.2	47
86	Spectroscopic accuracy directly from quantum chemistry: Application to ground and excited states of beryllium dimer. <i>Journal of Chemical Physics</i> , 2014, 140, 104112.	3.0	75
87	Low-energy spectrum of iron-sulfur clusters directly from many-particle quantum mechanics. <i>Nature Chemistry</i> , 2014, 6, 927-933.	13.6	227
88	Exact and Optimal Quantum Mechanics/Molecular Mechanics Boundaries. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3784-3790.	5.3	37
89	Ab initio determination of the crystalline benzene lattice energy to sub-kilojoule/mole accuracy. <i>Science</i> , 2014, 345, 640-643.	12.6	230
90	Thouless theorem for matrix product states and subsequent post density matrix renormalization group methods. <i>Physical Review B</i> , 2013, 88, .	3.2	38

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91	Entangled quantum electronic wavefunctions of the Mn ₄ CaO ₅ cluster in photosystem II. Nature Chemistry, 2013, 5, 660-666.	13.6	215
92	Density Matrix Embedding: A Strong-Coupling Quantum Embedding Theory. Journal of Chemical Theory and Computation, 2013, 9, 1428-1432.	5.3	238
93	Striped Spin Liquid Crystal Ground State Instability of Kagome Antiferromagnets. Physical Review Letters, 2013, 111, 187205.	7.8	34
94	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
95	Correlator product state study of molecular magnetism in the giant Keplerate Mo ₇₂ Fe ₃₀ . Physical Review B, 2012, 86, .	3.2	15
96	The orbital-specific-virtual local coupled cluster singles and doubles method. Journal of Chemical Physics, 2012, 136, 144105.	3.0	163
97	Excited States of Butadiene to Chemical Accuracy: Reconciling Theory and Experiment. Journal of Chemical Theory and Computation, 2012, 8, 4013-4018.	5.3	82
98	Density Matrix Embedding: A Simple Alternative to Dynamical Mean-Field Theory. Physical Review Letters, 2012, 109, 186404.	7.8	353
99	Spin-adapted density matrix renormalization group algorithms for quantum chemistry. Journal of Chemical Physics, 2012, 136, 124121.	3.0	229
100	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
101	The Density Matrix Renormalization Group in Quantum Chemistry. Annual Review of Physical Chemistry, 2011, 62, 465-481.	10.8	572
102	A review of canonical transformation theory. International Reviews in Physical Chemistry, 2010, 29, 231-271.	2.3	86
103	Quadratic canonical transformation theory and higher order density matrices. Journal of Chemical Physics, 2009, 130, 124102.	3.0	81
104	Analytic response theory for the density matrix renormalization group. Journal of Chemical Physics, 2009, 130, 184111.	3.0	55
105	A study of cumulant approximations to n-electron valence multireference perturbation theory. Journal of Chemical Physics, 2009, 130, 194107.	3.0	70
106	Accelerating convergence in iterative solution for large-scale complete active space self-consistent-field calculations. International Journal of Quantum Chemistry, 2009, 109, 2178-2190.	2.0	84
107	Chapter 7 The Density Matrix Renormalization Group in Quantum Chemistry. Annual Reports in Computational Chemistry, 2009, 5, 149-162.	1.7	72
108	Orbital optimization in the density matrix renormalization group, with applications to polyenes and β -carotene. Journal of Chemical Physics, 2008, 128, 144117.	3.0	288

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109	Density matrix renormalisation group Lagrangians. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 3454.	2.8	34
110	The radical character of the acenes: A density matrix renormalization group study. <i>Journal of Chemical Physics</i> , 2007, 127, 134309.	3.0	421
111	Canonical transformation theory from extended normal ordering. <i>Journal of Chemical Physics</i> , 2007, 127, 104107.	3.0	122
112	Canonical transformation theory for multireference problems. <i>Journal of Chemical Physics</i> , 2006, 124, 194106.	3.0	204
113	Tailored coupled cluster singles and doubles method applied to calculations on molecular structure and harmonic vibrational frequencies of ozone. <i>Journal of Chemical Physics</i> , 2006, 124, 114311.	3.0	80
114	Multireference correlation in long molecules with the quadratic scaling density matrix renormalization group. <i>Journal of Chemical Physics</i> , 2006, 125, 144101.	3.0	174
115	Density-matrix renormalization-group algorithms with nonorthogonal orbitals and non-Hermitian operators, and applications to polyenes. <i>Journal of Chemical Physics</i> , 2005, 122, 204101.	3.0	56
116	Time-Dependent Density Functional Theory of Classical Fluids. <i>Physical Review Letters</i> , 2005, 94, 183001.	7.8	64
117	An algorithm for large scale density matrix renormalization group calculations. <i>Journal of Chemical Physics</i> , 2004, 120, 3172-3178.	3.0	174
118	State-of-the-art density matrix renormalization group and coupled cluster theory studies of the nitrogen binding curve. <i>Journal of Chemical Physics</i> , 2004, 121, 6110-6116.	3.0	172
119	Exact solution (within a triple-zeta, double polarization basis set) of the electronic Schrödinger equation for water. <i>Journal of Chemical Physics</i> , 2003, 118, 8551-8554.	3.0	109
120	Highly correlated calculations with a polynomial cost algorithm: A study of the density matrix renormalization group. <i>Journal of Chemical Physics</i> , 2002, 116, 4462-4476.	3.0	459
121	Thomas-Fermi-Dirac-von Weizsäcker models in finite systems. <i>Journal of Chemical Physics</i> , 2001, 114, 631.	3.0	59
122	An extensive study of gradient approximations to the exchange-correlation and kinetic energy functionals. <i>Journal of Chemical Physics</i> , 2000, 112, 5639-5653.	3.0	43
123	A fresh look at ensembles: Derivative discontinuities in density functional theory. <i>Journal of Chemical Physics</i> , 1999, 110, 4710-4723.	3.0	73
124	Optimized Lieb-Oxford bound for the exchange-correlation energy. <i>Physical Review A</i> , 1999, 59, 3075-3077.	2.5	67
125	Kinetic-energy systems, density scaling, and homogeneity relations in density-functional theory. <i>Physical Review A</i> , 1999, 59, 2670-2679.	2.5	48
126	The Fermionic Quantum Emulator. <i>Quantum - the Open Journal for Quantum Science</i> , 0, 5, 568.	0.0	9