Lin Lin

List of Publications by Year
in descending order

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102	3,530	172386	155592
papers	citations	29 h-index	55 g-index

104	104	104	3589
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	GW100: Benchmarking G₀W₀ for Molecular Systems. Journal of Chemical Theory and Computation, 2015, 11, 5665-5687.	2.3	280
2	Highly Efficient Photocatalytic Water Splitting over Edge-Modified Phosphorene Nanoribbons. Journal of the American Chemical Society, 2017, 139, 15429-15436.	6.6	244
3	S<scp>iesta</scp>: Recent developments and applications. Journal of Chemical Physics, 2020, 152, 204108.	1.2	229
4	Edge-Modified Phosphorene Nanoflake Heterojunctions as Highly Efficient Solar Cells. Nano Letters, 2016, 16, 1675-1682.	4.5	176
5	SelInv---An Algorithm for Selected Inversion of a Sparse Symmetric Matrix. ACM Transactions on Mathematical Software, 2011, 37, 1-19.	1.6	167
6	Adaptive local basis set for Kohnâ€“Sham density functional theory in a discontinuous Galerkin framework I: Total energy calculation. Journal of Computational Physics, 2012, 231, 2140-2154.	1.9	162
7	Adaptively Compressed Exchange Operator. Journal of Chemical Theory and Computation, 2016, 12, 2242-2249.	2.3	118
8	86 PFLOPS Deep Potential Molecular Dynamics simulation of 100 million atoms with ab initio accuracy. Computer Physics Communications, 2021, 259, 107624.	3.0	100
9	Approximating Spectral Densities of Large Matrices. SIAM Review, 2016, 58, 34-65.	4.2	84
10	ELSI: A unified software interface for Kohnâ€“Sham electronic structure solvers. Computer Physics Communications, 2018, 222, 267-285.	3.0	78
11	Fast construction of hierarchical matrix representation from matrixâ€“vector multiplication. Journal of Computational Physics, 2011, 230, 4071-4087.	1.9	72
12	Compressed Representation of Kohnâ€“Sham Orbitals via Selected Columns of the Density Matrix. Journal of Chemical Theory and Computation, 2015, 11, 1463-1469.	2.3	72
13	Near-optimal ground state preparation. Quantum - the Open Journal for Quantum Science, 0, 4, 372.	0.0	64
14	Fast algorithm for extracting the diagonal of the inverse matrix with application to the electronic structure analysis of metallic systems. Communications in Mathematical Sciences, 2009, 7, 755-777.	0.5	59
15	DGDFT: A massively parallel method for large scale density functional theory calculations. Journal of Chemical Physics, 2015, 143, 124110.	1.2	55
16	Interpolative Separable Density Fitting Decomposition for Accelerating Hybrid Density Functional Calculations with Applications to Defects in Silicon. Journal of Chemical Theory and Computation, 2017, 13, 5420-5431.	2.3	53
17	Elliptic Preconditioner for Accelerating the Self-Consistent Field Iteration in Kohn--Sham Density Functional Theory. SIAM Journal of Scientific Computing, 2013, 35, S277-S298.	1.3	51
18	Accelerating atomic orbital-based electronic structure calculation via pole expansion and selected inversion. Journal of Physics Condensed Matter, 2013, 25, 295501.	0.7	50

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19	Displaced Path Integral Formulation for the Momentum Distribution of Quantum Particles. Physical Review Letters, 2010, 105, 110602.	2.9	49
20	Pole-Based approximation of the Fermi-Dirac function. Chinese Annals of Mathematics Series B, 2009, 30, 729-742.	0.2	46
21	Correlated Tunneling in Hydrogen Bonds. Journal of Statistical Physics, 2011, 145, 365-384.	0.5	45
22	Systematically Improvable Tensor Hypercontraction: Interpolative Separable Density-Fitting for Molecules Applied to Exact Exchange, Second- and Third-Order MÃ¸llerâ€“Plesset Perturbation Theory. Journal of Chemical Theory and Computation, 2020, 16, 243-263.	2.3	44
23	Optimal polynomial based quantum eigenstate filtering with application to solving quantum linear systems. Quantum - the Open Journal for Quantum Science, 0, 4, 361.	0.0	44
24	Electronic structure and aromaticity of large-scale hexagonal graphene nanoflakes. Journal of Chemical Physics, 2014, 141, 214704.	1.2	40
25	Heisenberg-Limited Ground-State Energy Estimation for Early Fault-Tolerant Quantum Computers. PRX Quantum, 2022, 3, .	3.5	40
26	Interpolative Separable Density Fitting through Centroidal Voronoi Tessellation with Applications to Hybrid Functional Electronic Structure Calculations. Journal of Chemical Theory and Computation, 2018, 14, 1311-1320.	2.3	39
27	Efficient phase-factor evaluation in quantum signal processing. Physical Review A, 2021, 103, .	1.0	39
28	Adaptively Compressed Exchange Operator for Large-Scale Hybrid Density Functional Calculations with Applications to the Adsorption of Water on Silicene. Journal of Chemical Theory and Computation, 2017, 13, 1188-1198.	2.3	38
29	Edge reconstruction in armchair phosphorene nanoribbons revealed by discontinuous Galerkin density functional theory. Physical Chemistry Chemical Physics, 2015, 17, 31397-31404.	1.3	37
30	SCDM-k: Localized orbitals for solids via selected columns of the density matrix. Journal of Computational Physics, 2017, 334, 1-15.	1.9	36
31	Fast inversion, preconditioned quantum linear system solvers, fast Green's-function computation, and fast evaluation of matrix functions. Physical Review A, 2021, 104, .	1.0	34
32	Momentum distribution, vibrational dynamics, and the potential of mean force in ice. Physical Review B, 2011, 83, .	1.1	33
33	Kantorovich dual solution for strictly correlated electrons in atoms and molecules. Physical Review B, 2013, 87, .	1.1	32
34	Adaptive local basis set for Kohnâ€“Sham density functional theory in a discontinuous Galerkin framework II: Force, vibration, and molecular dynamics calculations. Journal of Computational Physics, 2017, 335, 426-443.	1.9	29
35	Reinforcement Learning for Many-Body Ground-State Preparation Inspired by Counterdiabatic Driving. Physical Review X, 2021, 11, .	2.8	29
36	Chebyshev polynomial filtered subspace iteration in the discontinuous Galerkin method for large-scale electronic structure calculations. Journal of Chemical Physics, 2016, 145, 154101.	1.2	28

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37	Two-Level Chebyshev Filter Based Complementary Subspace Method: Pushing the Envelope of Large-Scale Electronic Structure Calculations. Journal of Chemical Theory and Computation, 2018, 14, 2930-2946.	2.3	28
38	Quantum Linear System Solver Based on Time-optimal Adiabatic Quantum Computing and Quantum Approximate Optimization Algorithm. ACM Transactions on Quantum Computing, 2022, 3, 1-28.	2.6	28
39	ELSI â€" An open infrastructure for electronic structure solvers. Computer Physics Communications, 2020, 256, 107459.	3.0	27
40	SIESTA-PEXSI: massively parallel method for efficient and accurateab initiomaterials simulation without matrix diagonalization. Journal of Physics Condensed Matter, 2014, 26, 305503.	0.7	25
41	Parallel eigenvalue calculation based on multiple shiftâ€"invert Lanczos and contour integral based spectral projection method. Parallel Computing, 2014, 40, 195-212.	1.3	25
42	Disentanglement via Entanglement: A Unified Method for Wannier Localization. Multiscale Modeling and Simulation, 2018, 16, 1392-1410.	0.6	25
43	Room-temperature magnetism and tunable energy gaps in edge-passivated zigzag graphene quantum dots. Npj 2D Materials and Applications, 2019, 3, .	3.9	25
44	Analysis of Time Reversible Born-Oppenheimer Molecular Dynamics. Entropy, 2014, 16, 110-137.	1.1	24
45	A Multiscale Neural Network Based on Hierarchical Matrices. Multiscale Modeling and Simulation, 2019, 17, 1189-1213.	0.6	24
46	Numerical methods for Kohnâ€"Sham density functional theory. Acta Numerica, 2019, 28, 405-539.	6.3	23
47	Time-dependent unbounded Hamiltonian simulation with vector norm scaling. Quantum - the Open Journal for Quantum Science, 0, 5, 459.	0.0	23
48	Adaptively Compressed Polarizability Operator for Accelerating Large Scale Ab Initio Phonon Calculations. Multiscale Modeling and Simulation, 2017, 15, 29-55.	0.6	22
49	Projected density matrix embedding theory with applications to the two-dimensional Hubbard model. Journal of Chemical Physics, 2019, 151, .	1.2	22
50	Projected Commutator DIIS Method for Accelerating Hybrid Functional Electronic Structure Calculations. Journal of Chemical Theory and Computation, 2017, 13, 5458-5467.	2.3	21
51	Fast Real-Time Time-Dependent Density Functional Theory Calculations with the Parallel Transport Gauge. Journal of Chemical Theory and Computation, 2018, 14, 5645-5652.	2.3	20
52	A multiscale neural network based on hierarchical nested bases. Research in Mathematical Sciences, 2019, 6, 1.	0.5	19
53	Structured Quasi-Newton Methods for Optimization with Orthogonality Constraints. SIAM Journal of Scientific Computing, 2019, 41, A2239-A2269.	1.3	18
54	Efficient hybridization fitting for dynamical mean-field theory via semi-definite relaxation. Physical Review B, 2020, 101, .	1.1	18

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55	Numerical integration for ab initio many-electron self energy calculations within the GW approximation. Journal of Computational Physics, 2015, 286, 1-13.	1.9	15
56	Low rank approximation in G 0 W 0 calculations. Science China Mathematics, 2016, 59, 1593-1612.	0.8	14
57	Influence of point defects on the electronic and topological properties of monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>WTe</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> Physical Review B, 2020, 102, .	1.1	14
58	Enhancing robustness and efficiency of density matrix embedding theory via semidefinite programming and local correlation potential fitting. Physical Review B, 2020, 102, .	1.1	13
59	Realizing Effective Cubic-Scaling Coulomb Hole Plus Screened Exchange Approximation in Periodic Systems via Interpolative Separable Density Fitting with a Plane-Wave Basis Set. Journal of Physical Chemistry A, 2021, 125, 7545-7557.	1.1	13
60	Accelerating Optical Absorption Spectra and Exciton Energy Computation via Interpolative Separable Density Fitting. Lecture Notes in Computer Science, 2018, , 604-617.	1.0	12
61	Discontinuous Galerkin discretization for quantum simulation of chemistry. New Journal of Physics, 2020, 22, 093015.	1.2	12
62	Fast real-time time-dependent hybrid functional calculations with the parallel transport gauge and the adaptively compressed exchange formulation. Computer Physics Communications, 2019, 240, 21-29.	3.0	11
63	Variational Formulation for Wannier Functions with Entangled Band Structure. Multiscale Modeling and Simulation, 2019, 17, 167-191.	0.6	11
64	Deep Density: Circumventing the Kohn-Sham equations via symmetry preserving neural networks. Journal of Computational Physics, 2021, 443, 110523.	1.9	11
65	Fast optical absorption spectra calculations for periodic solid state systems. Communications in Applied Mathematics and Computational Science, 2020, 15, 89-113.	0.7	10
66	A posteriori error estimator for adaptive local basis functions to solve Kohnâ€“Sham density functional theory. Communications in Mathematical Sciences, 2015, 13, 1741-1773.	0.5	10
67	Optimized local basis set for Kohnâ€“Sham density functional theory. Journal of Computational Physics, 2012, 231, 4515-4529.	1.9	9
68	Randomized estimation of spectral densities of large matrices made accurate. Numerische Mathematik, 2017, 136, 183-213.	0.9	9
69	KSSOLV 2.0: An efficient MATLAB toolbox for solving the Kohn-Sham equations with plane-wave basis set. Computer Physics Communications, 2022, 279, 108424.	3.0	9
70	Random circuit block-encoded matrix and a proposal of quantum LINPACK benchmark. Physical Review A, 2021, 103, .	1.0	8
71	Pure State v-Representability of Density Matrix Embedding Theory. Journal of Chemical Theory and Computation, 2022, 18, 851-864.	2.3	8
72	PSelInv â€“ A distributed memory parallel algorithm for selected inversion: The non-symmetric case. Parallel Computing, 2018, 74, 84-98.	1.3	7

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73	Convergence of Adaptive Compression Methods for Hartreeâ€Fockâ€Like Equations. Communications on Pure and Applied Mathematics, 2019, 72, 451-499.	1.2	7
74	Parallel transport time-dependent density functional theory calculations with hybrid functional on summit. , 2019, , .		7
75	Staggered Mesh Method for Correlation Energy Calculations of Solids: Random Phase Approximation in Direct Ring Coupled Cluster Doubles and Adiabatic Connection Formalisms. Journal of Chemical Theory and Computation, 2022, 18, 763-775.	2.3	7
76	Time-dependent Hamiltonian Simulation of Highly Oscillatory Dynamics and Superconvergence for SchrÃ¶dinger Equation. Quantum - the Open Journal for Quantum Science, 0, 6, 690.	0.0	7
77	A posteriorierror estimates for discontinuous Galerkin methods using non-polynomial basis functions Part I: Second order linear PDE. ESAIM: Mathematical Modelling and Numerical Analysis, 2016, 50, 1193-1222.	0.8	6
78	Staggered Mesh Method for Correlation Energy Calculations of Solids: Second-Order MÃ¸llerâ€“Plesset Perturbation Theory. Journal of Chemical Theory and Computation, 2021, 17, 4733-4745.	2.3	6
79	Element orbitals for Kohn-Sham density functional theory. Physical Review B, 2012, 85, .	1.1	5
80	Decay estimates of discretized Greenâ€™s functions for SchrÃ¶dinger type operators. Science China Mathematics, 2016, 59, 1561-1578.	0.8	5
81	Robust determination of the chemical potential in the pole expansion and selected inversion method for solving Kohn-Sham density functional theory. Journal of Chemical Physics, 2017, 147, 144107.	1.2	5
82	Variational structure of Luttingerâ€“Ward formalism and bold diagrammatic expansion for Euclidean lattice field theory. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 2282-2286.	3.3	5
83	Stochastic Constrained Extended System Dynamics for Solving Charge Equilibration Models. Journal of Chemical Theory and Computation, 2020, 16, 5991-5998.	2.3	5
84	Semidefinite Relaxation of Multimarginal Optimal Transport for Strictly Correlated Electrons in Second Quantization. SIAM Journal of Scientific Computing, 2020, 42, B1462-B1489.	1.3	5
85	Localized spectrum slicing. Mathematics of Computation, 2017, 86, 2345-2371.	1.1	4
86	A posteriorierror estimates for discontinuous Galerkin methods using non-polynomial basis functions. Part II: Eigenvalue problems. ESAIM: Mathematical Modelling and Numerical Analysis, 2017, 51, 1733-1753.	0.8	4
87	PEXSI-$Sigma$: a Greenâ€™s function embedding method for Kohnâ€“Sham density functional theory. Annals of Mathematical Sciences and Applications, 2018, 3, 441-472.	0.2	4
88	Universal approximation of symmetric and anti-symmetric functions. Communications in Mathematical Sciences, 2022, 20, 1397-1408.	0.5	4
89	Quantum Dynamics with the Parallel Transport Gauge. Multiscale Modeling and Simulation, 2020, 18, 612-645.	0.6	3
90	Mesh independence of the generalized Davidson algorithm. Journal of Computational Physics, 2020, 409, 109322.	1.9	3

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91	Low-Rank Representation of Tensor Network Operators with Long-Range Pairwise Interactions. SIAM Journal of Scientific Computing, 2021, 43, A164-A192.	1.3	3
92	Variational Embedding for Quantum Manyâ€Body Problems. Communications on Pure and Applied Mathematics, 0, , .	1.2	3
93	Numerical solution of large scale Hartreeâ€“Fockâ€“Bogoliubov equations. ESAIM: Mathematical Modelling and Numerical Analysis, 2021, 55, 763-787.	0.8	3
94	Split representation of adaptively compressed polarizability operator. Research in Mathematical Sciences, 2021, 8, 1.	0.5	3
95	Convergence of stochastic-extended Lagrangian molecular dynamics method for polarizable force field simulation. Journal of Computational Physics, 2021, 438, 110338.	1.9	3
96	Globally Constructed Adaptive Local Basis Set for Spectral Projectors of Second Order Differential Operators. Multiscale Modeling and Simulation, 2019, 17, 92-116.	0.6	2
97	Parallel transport dynamics for mixed quantum states with applications to time-dependent density functional theory. Journal of Computational Physics, 2022, 451, 110850.	1.9	2
98	Sparsity Pattern of the Self-energy for Classical and Quantum Impurity Problems. Annales Henri Poincare, 2020, 21, 2219-2257.	0.8	1
99	Learning the Mapping $$mathbf {x}mapsto sumlimits _{i=1}^d x_i^2$$: the Cost of Finding the Needle in a Haystack. Communications on Applied Mathematics and Computation, 2021, 3, 313-335.	0.7	1
100	Bold Feynman Diagrams and the Luttingerâ€“Ward Formalism Via Gibbs Measures: Non-perturbative Analysis. Archive for Rational Mechanics and Analysis, 2021, 242, 527-579.	1.1	1
101	Bold Feynman Diagrams and the Luttingerâ€“Ward Formalism via Gibbs Measures: Perturbative Approach. Archive for Rational Mechanics and Analysis, 2021, 242, 581-642.	1.1	1
102	Towards sharp error analysis of extended Lagrangian molecular dynamics. Journal of Computational Physics, 2022, 466, 111403.	1.9	0