

Lin Lin

List of Publications by Year in descending order

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102
papers

3,530
citations

172457

29
h-index

155660

55
g-index

104
all docs

104
docs citations

104
times ranked

3589
citing authors

#	ARTICLE	IF	CITATIONS
1	<i>GW</i> 100: Benchmarking <i>G</i> ₀ <i>W</i> ₀ for Molecular Systems. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5665-5687.	5.3	280
2	Highly Efficient Photocatalytic Water Splitting over Edge-Modified Phosphorene Nanoribbons. <i>Journal of the American Chemical Society</i> , 2017, 139, 15429-15436.	13.7	244
3	<i>Scipy</i> : Recent developments and applications. <i>Journal of Chemical Physics</i> , 2020, 152, 204108.	3.0	229
4	Edge-Modified Phosphorene Nanoflake Heterojunctions as Highly Efficient Solar Cells. <i>Nano Letters</i> , 2016, 16, 1675-1682.	9.1	176
5	<i>Selln</i> --An Algorithm for Selected Inversion of a Sparse Symmetric Matrix. <i>ACM Transactions on Mathematical Software</i> , 2011, 37, 1-19.	2.9	167
6	Adaptive local basis set for Kohn-Sham density functional theory in a discontinuous Galerkin framework I: Total energy calculation. <i>Journal of Computational Physics</i> , 2012, 231, 2140-2154.	3.8	162
7	Adaptively Compressed Exchange Operator. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2242-2249.	5.3	118
8	86 PFLOPS Deep Potential Molecular Dynamics simulation of 100 million atoms with ab initio accuracy. <i>Computer Physics Communications</i> , 2021, 259, 107624.	7.5	100
9	Approximating Spectral Densities of Large Matrices. <i>SIAM Review</i> , 2016, 58, 34-65.	9.5	84
10	ELSI: A unified software interface for Kohn-Sham electronic structure solvers. <i>Computer Physics Communications</i> , 2018, 222, 267-285.	7.5	78
11	Fast construction of hierarchical matrix representation from matrix-vector multiplication. <i>Journal of Computational Physics</i> , 2011, 230, 4071-4087.	3.8	72
12	Compressed Representation of Kohn-Sham Orbitals via Selected Columns of the Density Matrix. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1463-1469.	5.3	72
13	Near-optimal ground state preparation. <i>Quantum - the Open Journal for Quantum Science</i> , 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. <i>Communications in Mathematical Sciences</i> , 2009, 7, 755-777.	1.0	59
15	DGDFT: A massively parallel method for large scale density functional theory calculations. <i>Journal of Chemical Physics</i> , 2015, 143, 124110.	3.0	55
16	Interpolative Separable Density Fitting Decomposition for Accelerating Hybrid Density Functional Calculations with Applications to Defects in Silicon. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5420-5431.	5.3	53
17	Elliptic Preconditioner for Accelerating the Self-Consistent Field Iteration in Kohn-Sham Density Functional Theory. <i>SIAM Journal of Scientific Computing</i> , 2013, 35, S277-S298.	2.8	51
18	Accelerating atomic orbital-based electronic structure calculation via pole expansion and selected inversion. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 295501.	1.8	50

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19	Displaced Path Integral Formulation for the Momentum Distribution of Quantum Particles. <i>Physical Review Letters</i> , 2010, 105, 110602.	7.8	49
20	Pole-Based approximation of the Fermi-Dirac function. <i>Chinese Annals of Mathematics Series B</i> , 2009, 30, 729-742.	0.4	46
21	Correlated Tunneling in Hydrogen Bonds. <i>Journal of Statistical Physics</i> , 2011, 145, 365-384.	1.2	45
22	Systematically Improvable Tensor Hypercontraction: Interpolative Separable Density-Fitting for Molecules Applied to Exact Exchange, Second- and Third-Order Møller-Plesset Perturbation Theory. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 243-263.	5.3	44
23	Optimal polynomial based quantum eigenstate filtering with application to solving quantum linear systems. <i>Quantum - the Open Journal for Quantum Science</i> , 0, 4, 361.	0.0	44
24	Electronic structure and aromaticity of large-scale hexagonal graphene nanoflakes. <i>Journal of Chemical Physics</i> , 2014, 141, 214704.	3.0	40
25	Heisenberg-Limited Ground-State Energy Estimation for Early Fault-Tolerant Quantum Computers. <i>PRX Quantum</i> , 2022, 3, .	9.2	40
26	Interpolative Separable Density Fitting through Centroidal Voronoi Tessellation with Applications to Hybrid Functional Electronic Structure Calculations. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1311-1320.	5.3	39
27	Efficient phase-factor evaluation in quantum signal processing. <i>Physical Review A</i> , 2021, 103, .	2.5	39
28	Adaptively Compressed Exchange Operator for Large-Scale Hybrid Density Functional Calculations with Applications to the Adsorption of Water on Silicene. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1188-1198.	5.3	38
29	Edge reconstruction in armchair phosphorene nanoribbons revealed by discontinuous Galerkin density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 31397-31404.	2.8	37
30	SCDM-k: Localized orbitals for solids via selected columns of the density matrix. <i>Journal of Computational Physics</i> , 2017, 334, 1-15.	3.8	36
31	Fast inversion, preconditioned quantum linear system solvers, fast Green's-function computation, and fast evaluation of matrix functions. <i>Physical Review A</i> , 2021, 104, .	2.5	34
32	Momentum distribution, vibrational dynamics, and the potential of mean force in ice. <i>Physical Review B</i> , 2011, 83, .	3.2	33
33	Kantorovich dual solution for strictly correlated electrons in atoms and molecules. <i>Physical Review B</i> , 2013, 87, .	3.2	32
34	Adaptive local basis set for Kohn-Sham density functional theory in a discontinuous Galerkin framework II: Force, vibration, and molecular dynamics calculations. <i>Journal of Computational Physics</i> , 2017, 335, 426-443.	3.8	29
35	Reinforcement Learning for Many-Body Ground-State Preparation Inspired by Counterdiabatic Driving. <i>Physical Review X</i> , 2021, 11, .	8.9	29
36	Chebyshev polynomial filtered subspace iteration in the discontinuous Galerkin method for large-scale electronic structure calculations. <i>Journal of Chemical Physics</i> , 2016, 145, 154101.	3.0	28

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37	Two-Level Chebyshev Filter Based Complementary Subspace Method: Pushing the Envelope of Large-Scale Electronic Structure Calculations. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2930-2946.	5.3	28
38	Quantum Linear System Solver Based on Time-optimal Adiabatic Quantum Computing and Quantum Approximate Optimization Algorithm. <i>ACM Transactions on Quantum Computing</i> , 2022, 3, 1-28.	4.3	28
39	ELSI – An open infrastructure for electronic structure solvers. <i>Computer Physics Communications</i> , 2020, 256, 107459.	7.5	27
40	SIESTA-PEXSI: massively parallel method for efficient and accurate <i>ab initio</i> materials simulation without matrix diagonalization. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 305503.	1.8	25
41	Parallel eigenvalue calculation based on multiple shift–invert Lanczos and contour integral based spectral projection method. <i>Parallel Computing</i> , 2014, 40, 195-212.	2.1	25
42	Disentanglement via Entanglement: A Unified Method for Wannier Localization. <i>Multiscale Modeling and Simulation</i> , 2018, 16, 1392-1410.	1.6	25
43	Room-temperature magnetism and tunable energy gaps in edge-passivated zigzag graphene quantum dots. <i>Npj 2D Materials and Applications</i> , 2019, 3, .	7.9	25
44	Analysis of Time Reversible Born-Oppenheimer Molecular Dynamics. <i>Entropy</i> , 2014, 16, 110-137.	2.2	24
45	A Multiscale Neural Network Based on Hierarchical Matrices. <i>Multiscale Modeling and Simulation</i> , 2019, 17, 1189-1213.	1.6	24
46	Numerical methods for Kohn–Sham density functional theory. <i>Acta Numerica</i> , 2019, 28, 405-539.	10.7	23
47	Time-dependent unbounded Hamiltonian simulation with vector norm scaling. <i>Quantum - the Open Journal for Quantum Science</i> , 0, 5, 459.	0.0	23
48	Adaptively Compressed Polarizability Operator for Accelerating Large Scale <i>Ab Initio</i> Phonon Calculations. <i>Multiscale Modeling and Simulation</i> , 2017, 15, 29-55.	1.6	22
49	Projected density matrix embedding theory with applications to the two-dimensional Hubbard model. <i>Journal of Chemical Physics</i> , 2019, 151, .	3.0	22
50	Projected Commutator DIIS Method for Accelerating Hybrid Functional Electronic Structure Calculations. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5458-5467.	5.3	21
51	Fast Real-Time Time-Dependent Density Functional Theory Calculations with the Parallel Transport Gauge. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 5645-5652.	5.3	20
52	A multiscale neural network based on hierarchical nested bases. <i>Research in Mathematical Sciences</i> , 2019, 6, 1.	1.0	19
53	Structured Quasi-Newton Methods for Optimization with Orthogonality Constraints. <i>SIAM Journal of Scientific Computing</i> , 2019, 41, A2239-A2269.	2.8	18
54	Efficient hybridization fitting for dynamical mean-field theory via semi-definite relaxation. <i>Physical Review B</i> , 2020, 101, .	3.2	18

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55	Numerical integration for ab initio many-electron self energy calculations within the GW approximation. <i>Journal of Computational Physics</i> , 2015, 286, 1-13.	3.8	15
56	Low rank approximation in G ₀ W ₀ calculations. <i>Science China Mathematics</i> , 2016, 59, 1593-1612.	1.7	14
57	Influence of point defects on the electronic and topological properties of monolayer WTe_2 . <i>Physical Review B</i> , 2020, 102, .		
58	Enhancing robustness and efficiency of density matrix embedding theory via semidefinite programming and local correlation potential fitting. <i>Physical Review B</i> , 2020, 102, .	3.2	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. <i>Journal of Physical Chemistry A</i> , 2021, 125, 7545-7557.	2.5	13
60	Accelerating Optical Absorption Spectra and Exciton Energy Computation via Interpolative Separable Density Fitting. <i>Lecture Notes in Computer Science</i> , 2018, , 604-617.	1.3	12
61	Discontinuous Galerkin discretization for quantum simulation of chemistry. <i>New Journal of Physics</i> , 2020, 22, 093015.	2.9	12
62	Fast real-time time-dependent hybrid functional calculations with the parallel transport gauge and the adaptively compressed exchange formulation. <i>Computer Physics Communications</i> , 2019, 240, 21-29.	7.5	11
63	Variational Formulation for Wannier Functions with Entangled Band Structure. <i>Multiscale Modeling and Simulation</i> , 2019, 17, 167-191.	1.6	11
64	Deep Density: Circumventing the Kohn-Sham equations via symmetry preserving neural networks. <i>Journal of Computational Physics</i> , 2021, 443, 110523.	3.8	11
65	Fast optical absorption spectra calculations for periodic solid state systems. <i>Communications in Applied Mathematics and Computational Science</i> , 2020, 15, 89-113.	1.8	10
66	<i>a posteriori</i> error estimator for adaptive local basis functions to solve Kohn-Sham density functional theory. <i>Communications in Mathematical Sciences</i> , 2015, 13, 1741-1773.	1.0	10
67	Optimized local basis set for Kohn-Sham density functional theory. <i>Journal of Computational Physics</i> , 2012, 231, 4515-4529.	3.8	9
68	Randomized estimation of spectral densities of large matrices made accurate. <i>Numerische Mathematik</i> , 2017, 136, 183-213.	1.9	9
69	KSSOLV 2.0: An efficient MATLAB toolbox for solving the Kohn-Sham equations with plane-wave basis set. <i>Computer Physics Communications</i> , 2022, 279, 108424.	7.5	9
70	Random circuit block-encoded matrix and a proposal of quantum LINPACK benchmark. <i>Physical Review A</i> , 2021, 103, .	2.5	8
71	Pure State $\langle i \nu \rangle \langle i $ -Representability of Density Matrix Embedding Theory. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 851-864.	5.3	8
72	PSellv: A distributed memory parallel algorithm for selected inversion: The non-symmetric case. <i>Parallel Computing</i> , 2018, 74, 84-98.	2.1	7

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73	Convergence of Adaptive Compression Methods for Hartree-Fock-Like Equations. <i>Communications on Pure and Applied Mathematics</i> , 2019, 72, 451-499.	3.1	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. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 763-775.	5.3	7
76	Time-dependent Hamiltonian Simulation of Highly Oscillatory Dynamics and Superconvergence for Schrödinger Equation. <i>Quantum - the Open Journal for Quantum Science</i> , 0, 6, 690.	0.0	7
77	A posteriori error estimates for discontinuous Galerkin methods using non-polynomial basis functions Part I: Second order linear PDE. <i>ESAIM: Mathematical Modelling and Numerical Analysis</i> , 2016, 50, 1193-1222.	1.9	6
78	Staggered Mesh Method for Correlation Energy Calculations of Solids: Second-Order Møller-Plesset Perturbation Theory. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4733-4745.	5.3	6
79	Element orbitals for Kohn-Sham density functional theory. <i>Physical Review B</i> , 2012, 85, .	3.2	5
80	Decay estimates of discretized Green's functions for Schrödinger type operators. <i>Science China Mathematics</i> , 2016, 59, 1561-1578.	1.7	5
81	Robust determination of the chemical potential in the pole expansion and selected inversion method for solving Kohn-Sham density functional theory. <i>Journal of Chemical Physics</i> , 2017, 147, 144107.	3.0	5
82	Variational structure of Luttinger-Ward formalism and bold diagrammatic expansion for Euclidean lattice field theory. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 2282-2286.	7.1	5
83	Stochastic Constrained Extended System Dynamics for Solving Charge Equilibration Models. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 5991-5998.	5.3	5
84	Semidefinite Relaxation of Multimarginal Optimal Transport for Strictly Correlated Electrons in Second Quantization. <i>SIAM Journal of Scientific Computing</i> , 2020, 42, B1462-B1489.	2.8	5
85	Localized spectrum slicing. <i>Mathematics of Computation</i> , 2017, 86, 2345-2371.	2.1	4
86	A posteriori error estimates for discontinuous Galerkin methods using non-polynomial basis functions. Part II: Eigenvalue problems. <i>ESAIM: Mathematical Modelling and Numerical Analysis</i> , 2017, 51, 1733-1753.	1.9	4
87	PEXSI- Σ : a Green's function embedding method for Kohn-Sham density functional theory. <i>Annals of Mathematical Sciences and Applications</i> , 2018, 3, 441-472.	0.4	4
88	Universal approximation of symmetric and anti-symmetric functions. <i>Communications in Mathematical Sciences</i> , 2022, 20, 1397-1408.	1.0	4
89	Quantum Dynamics with the Parallel Transport Gauge. <i>Multiscale Modeling and Simulation</i> , 2020, 18, 612-645.	1.6	3
90	Mesh independence of the generalized Davidson algorithm. <i>Journal of Computational Physics</i> , 2020, 409, 109322.	3.8	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.	2.8	3
92	Variational Embedding for Quantum Many-Body Problems. Communications on Pure and Applied Mathematics, 0, , .	3.1	3
93	Numerical solution of large scale Hartree-Fock-Bogoliubov equations. ESAIM: Mathematical Modelling and Numerical Analysis, 2021, 55, 763-787.	1.9	3
94	Split representation of adaptively compressed polarizability operator. Research in Mathematical Sciences, 2021, 8, 1.	1.0	3
95	Convergence of stochastic-extended Lagrangian molecular dynamics method for polarizable force field simulation. Journal of Computational Physics, 2021, 438, 110338.	3.8	3
96	Globally Constructed Adaptive Local Basis Set for Spectral Projectors of Second Order Differential Operators. Multiscale Modeling and Simulation, 2019, 17, 92-116.	1.6	2
97	Parallel transport dynamics for mixed quantum states with applications to time-dependent density functional theory. Journal of Computational Physics, 2022, 451, 110850.	3.8	2
98	Sparsity Pattern of the Self-energy for Classical and Quantum Impurity Problems. Annales Henri Poincare, 2020, 21, 2219-2257.	1.7	1
99	Learning the Mapping $\mathbf{x} \mapsto \sum_{i=1}^d x_i^2$: the Cost of Finding the Needle in a Haystack. Communications on Applied Mathematics and Computation, 2021, 3, 313-335.	1.7	1
100	Bold Feynman Diagrams and the Luttinger-Ward Formalism Via Gibbs Measures: Non-perturbative Analysis. Archive for Rational Mechanics and Analysis, 2021, 242, 527-579.	2.4	1
101	Bold Feynman Diagrams and the Luttinger-Ward Formalism via Gibbs Measures: Perturbative Approach. Archive for Rational Mechanics and Analysis, 2021, 242, 581-642.	2.4	1
102	Towards sharp error analysis of extended Lagrangian molecular dynamics. Journal of Computational Physics, 2022, 466, 111403.	3.8	0