Chao Yang

List of Publications by Year in Descending Order

63 papers	1,706 citations	22 h-index	40 g-index
64 ext. papers	2,022 ext. citations	4.6 avg, IF	4.96 L-index

#	Paper	IF	Citations
63	Low rank approximation in simulations of quantum algorithms. *Journal of Computational Science*, **2022**, 59, 101561	3.4	
62	Accelerating an iterative eigensolver for nuclear structure configuration interaction calculations on GPUs using OpenACC. *Journal of Computational Science*, **2022**, 59, 101554	3.4	1
61	Accelerating Quantum Many-Body Configuration Interaction with Directives. *Lecture Notes in Computer Science*, **2022**, 112-132	0.9	
60	KSSOLV 2.0: An efficient MATLAB toolbox for solving the Kohn-Sham equations with plane-wave basis set. *Computer Physics Communications*, **2022**, 108424	4.2	2
59	From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape. *Chemical Reviews*, **2021**, 121, 4962-4998	68.1	12
58	Quantum Fourier transform revisited. *Numerical Linear Algebra With Applications*, **2021**, 28,	1.6	1
57	A greedy algorithm for computing eigenvalues of a symmetric matrix with localized eigenvectors. *Numerical Linear Algebra With Applications*, **2021**, 28, e2341	1.6	2
56	Reinforcement Learning Configuration Interaction. *Journal of Chemical Theory and Computation*, **2021**, 17, 5482-5491	6.4	1
55	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	2.8	4
54	ELSI An open infrastructure for electronic structure solvers. *Computer Physics Communications*, **2020**, 256, 107459	4.2	14
53	Scalable implementation of polynomial filtering for density functional theory calculation in PARSEC. *Computer Physics Communications*, **2020**, 254, 107330	4.2	4
52	Mesh independence of the generalized Davidson algorithm. *Journal of Computational Physics*, **2020**, 409, 109322	4.1	1
51	A Scalable Matrix-Free Iterative Eigensolver for Studying Many-Body Localization **2020**,		2
50	A Shift Selection Strategy for Parallel Shift-invert Spectrum Slicing in Symmetric Self-consistent Eigenvalue Computation. *ACM Transactions on Mathematical Software*, **2020**, 46, 1-31	2.3	1
49	Computing the density of states for optical spectra of molecules by low-rank and QTT tensor approximation. *Journal of Computational Physics*, **2019**, 382, 221-239	4.1	
48	Approximate Green's Function Coupled Cluster Method Employing Effective Dimension Reduction. *Journal of Chemical Theory and Computation*, **2019**, 15, 3185-3196	6.4	12
47	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	6.4	18

46	PSelInv – A distributed memory parallel algorithm for selected inversion: The non-symmetric case. *Parallel Computing*, **2018**, 74, 84-98	1	6
45	ELSI: A unified software interface for Kohn–Sham electronic structure solvers. *Computer Physics Communications*, **2018**, 222, 267-285	4.2	43
44	Accelerating nuclear configuration interaction calculations through a preconditioned block iterative eigensolver. *Computer Physics Communications*, **2018**, 222, 1-13	4.2	22
43	Optimized Pair Natural Orbitals for the Coupled Cluster Methods. *Journal of Chemical Theory and Computation*, **2018**, 14, 4581-4589	6.4	11
42	Computing resonant modes of accelerator cavities by solving nonlinear eigenvalue problems via rational approximation. *Journal of Computational Physics*, **2018**, 374, 1031-1043	4.1	7
41	Accelerating Optical Absorption Spectra and Exciton Energy Computation via Interpolative Separable Density Fitting. *Lecture Notes in Computer Science*, **2018**, 604-617	0.9	9
40	Some remarks on the complex J-symmetric eigenproblem. *Linear Algebra and Its Applications*, **2018**, 544, 407-442	0.9	9
39	A Structure Preserving Lanczos Algorithm for Computing the Optical Absorption Spectrum. *SIAM Journal on Matrix Analysis and Applications*, **2018**, 39, 683-711	1.5	10
38	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	6.4	21
37	Adaptive local basis set for Kohn–Sham density functional theory in a discontinuous Galerkin framework II: Force, vibration, and molecular dynamics calculations. *Journal of Computational Physics*, **2017**, 335, 426-443	4.1	19
36	Highly Efficient Photocatalytic Water Splitting over Edge-Modified Phosphorene Nanoribbons. *Journal of the American Chemical Society*, **2017**, 139, 15429-15436	16.4	176
35	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	6.4	29
34	Model Order Reduction Algorithm for Estimating the Absorption Spectrum. *Journal of Chemical Theory and Computation*, **2017**, 13, 4950-4961	6.4	11
33	Projected Commutator DIIS Method for Accelerating Hybrid Functional Electronic Structure Calculations. *Journal of Chemical Theory and Computation*, **2017**, 13, 5458-5467	6.4	15
32	Properties of Definite Bethe–Salpeter Eigenvalue Problems. *Lecture Notes in Computational Science and Engineering*, **2017**, 91-105	0.3	
31	molgw 1: Many-body perturbation theory software for atoms, molecules, and clusters. *Computer Physics Communications*, **2016**, 208, 149-161	4.2	97
30	Trace-Penalty Minimization for Large-Scale Eigenspace Computation. *Journal of Scientific Computing*, **2016**, 66, 1175-1203	2.3	17
29	Approximating Spectral Densities of Large Matrices. *SIAM Review*, **2016**, 58, 34-65	7.4	56

28	Edge-Modified Phosphorene Nanoflake Heterojunctions as Highly Efficient Solar Cells. *Nano Letters* , **2016**, 16, 1675-82	11.5	142
27	Structure preserving parallel algorithms for solving the Bethe‐Salpeter eigenvalue problem. *Linear Algebra and Its Applications*, **2016**, 488, 148-167	0.9	31
26	Low rank approximation in G 0 W 0 calculations. *Science China Mathematics*, **2016**, 59, 1593-1612	0.8	10
25	Chebyshev polynomial filtered subspace iteration in the discontinuous Galerkin method for large-scale electronic structure calculations. *Journal of Chemical Physics*, **2016**, 145, 154101	3.9	21
24	Edge reconstruction in armchair phosphorene nanoribbons revealed by discontinuous Galerkin density functional theory. *Physical Chemistry Chemical Physics*, **2015**, 17, 31397-404	3.6	34
23	GW100: Benchmarking G0W0 for Molecular Systems. *Journal of Chemical Theory and Computation*, **2015**, 11, 5665-87	6.4	207
22	Efficient Algorithms for Estimating the Absorption Spectrum within Linear Response TDDFT. *Journal of Chemical Theory and Computation*, **2015**, 11, 5197-208	6.4	25
21	New algorithms for iterative matrix-free eigensolvers in quantum chemistry. *Journal of Computational Chemistry*, **2015**, 36, 273-84	3.5	34
20	DGDFT: A massively parallel method for large scale density functional theory calculations. *Journal of Chemical Physics*, **2015**, 143, 124110	3.9	42
19	Numerical integration for ab initio many-electron self energy calculations within the GW approximation. *Journal of Computational Physics*, **2015**, 286, 1-13	4.1	11
18	A posteriori error estimator for adaptive local basis functions to solve Kohn‐Sham density functional theory. *Communications in Mathematical Sciences*, **2015**, 13, 1741-1773	1	9
17	Improving the scalability of a symmetric iterative eigensolver for multi-core platforms. *Concurrency Computation Practice and Experience*, **2014**, 26, 2631-2651	1.4	46
16	SIESTA-PEXSI: massively parallel method for efficient and accurate ab initio materials simulation without matrix diagonalization. *Journal of Physics Condensed Matter*, **2014**, 26, 305503	1.8	22
15	Electronic structure and aromaticity of large-scale hexagonal graphene nanoflakes. *Journal of Chemical Physics*, **2014**, 141, 214704	3.9	38
14	Accelerating atomic orbital-based electronic structure calculation via pole expansion and selected inversion. *Journal of Physics Condensed Matter*, **2013**, 25, 295501	1.8	41
13	Elliptic Preconditioner for Accelerating the Self-Consistent Field Iteration in Kohn--Sham Density Functional Theory. *SIAM Journal of Scientific Computing*, **2013**, 35, S277-S298	2.6	37
12	Minimizing the Kohn‐Sham total energy for periodic systems. *Linear Algebra and Its Applications*, **2012**, 436, 2764-2779	0.9	
11	SelInv---An Algorithm for Selected Inversion of a Sparse Symmetric Matrix. *ACM Transactions on Mathematical Software*, **2011**, 37, 1-19	2.3	133

10	KSSOLV– MATLAB toolbox for solving the Kohn-Sham equations. *ACM Transactions on Mathematical Software*, **2009**, 36, 1-35	2.3	64
9	Accelerating configuration interaction calculations for nuclear structure **2008**,		22
8	The parallelization of SPIDER on distributed-memory computers using MPI. *Journal of Structural Biology*, **2007**, 157, 240-9	3.4	12
7	A Trust Region Direct Constrained Minimization Algorithm for the Kohn–Sham Equation. *SIAM Journal of Scientific Computing*, **2007**, 29, 1854-1875	2.6	45
6	A constrained optimization algorithm for total energy minimization in electronic structure calculations. *Journal of Computational Physics*, **2006**, 217, 709-721	4.1	37
5	Matrix-free constructions of circulant and block circulant preconditioners. *Numerical Linear Algebra With Applications*, **2004**, 11, 773-793	1.6	1
4	Computational simulation of polymer particle structures: vibrational normal modes using the time averaged normal coordinate analysis method. *Polymer*, **2003**, 44, 3761-3767	3.9	3
3	Normal Coordinate Analysis for Polymer Systems: Capabilities and New Opportunities. *Macromolecular Theory and Simulations*, **2002**, 11, 711-728	1.5	2
2	Large-Scale Normal Coordinate Analysis on Distributed Memory Parallel Systems. *International Journal of High Performance Computing Applications*, **2002**, 16, 409-424	1.8	1
1	An Efficient Algorithm for Calculating the Heat Capacity of a Large-Scale Molecular System. *Macromolecular Theory and Simulations*, **2001**, 10, 756-761	1.5	2