

Chao Yang

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	GW100: Benchmarking G0W0 for Molecular Systems. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 5665-87	6.4	207
62	Highly Efficient Photocatalytic Water Splitting over Edge-Modified Phosphorene Nanoribbons. <i>Journal of the American Chemical Society</i> , 2017 , 139, 15429-15436	16.4	176
61	Edge-Modified Phosphorene Nanoflake Heterojunctions as Highly Efficient Solar Cells. <i>Nano Letters</i> , 2016 , 16, 1675-82	11.5	142
60	SellInv---An Algorithm for Selected Inversion of a Sparse Symmetric Matrix. <i>ACM Transactions on Mathematical Software</i> , 2011 , 37, 1-19	2.3	133
59	molgw 1: Many-body perturbation theory software for atoms, molecules, and clusters. <i>Computer Physics Communications</i> , 2016 , 208, 149-161	4.2	97
58	KSSOLV MATLAB toolbox for solving the Kohn-Sham equations. <i>ACM Transactions on Mathematical Software</i> , 2009 , 36, 1-35	2.3	64
57	Approximating Spectral Densities of Large Matrices. <i>SIAM Review</i> , 2016 , 58, 34-65	7.4	56
56	Improving the scalability of a symmetric iterative eigensolver for multi-core platforms. <i>Concurrency Computation Practice and Experience</i> , 2014 , 26, 2631-2651	1.4	46
55	A Trust Region Direct Constrained Minimization Algorithm for the Kohn-Sham Equation. <i>SIAM Journal of Scientific Computing</i> , 2007 , 29, 1854-1875	2.6	45
54	ELSI: A unified software interface for Kohn-Sham electronic structure solvers. <i>Computer Physics Communications</i> , 2018 , 222, 267-285	4.2	43
53	DGDFT: A massively parallel method for large scale density functional theory calculations. <i>Journal of Chemical Physics</i> , 2015 , 143, 124110	3.9	42
52	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	41
51	Electronic structure and aromaticity of large-scale hexagonal graphene nanoflakes. <i>Journal of Chemical Physics</i> , 2014 , 141, 214704	3.9	38
50	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	2.6	37
49	A constrained optimization algorithm for total energy minimization in electronic structure calculations. <i>Journal of Computational Physics</i> , 2006 , 217, 709-721	4.1	37
48	Edge reconstruction in armchair phosphorene nanoribbons revealed by discontinuous Galerkin density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 31397-404	3.6	34
47	New algorithms for iterative matrix-free eigensolvers in quantum chemistry. <i>Journal of Computational Chemistry</i> , 2015 , 36, 273-84	3.5	34

46	Structure preserving parallel algorithms for solving the Bethe-Balpeter eigenvalue problem. <i>Linear Algebra and Its Applications</i> , 2016 , 488, 148-167	0.9	31
45	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	6.4	29
44	Efficient Algorithms for Estimating the Absorption Spectrum within Linear Response TDDFT. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 5197-208	6.4	25
43	Accelerating nuclear configuration interaction calculations through a preconditioned block iterative eigensolver. <i>Computer Physics Communications</i> , 2018 , 222, 1-13	4.2	22
42	SIESTA-PEXSI: massively parallel method for efficient and accurate ab initio materials simulation without matrix diagonalization. <i>Journal of Physics Condensed Matter</i> , 2014 , 26, 305503	1.8	22
41	Accelerating configuration interaction calculations for nuclear structure 2008 ,		22
40	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	6.4	21
39	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	3.9	21
38	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	4.1	19
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	6.4	18
36	Trace-Penalty Minimization for Large-Scale Eigenspace Computation. <i>Journal of Scientific Computing</i> , 2016 , 66, 1175-1203	2.3	17
35	Projected Commutator DIIS Method for Accelerating Hybrid Functional Electronic Structure Calculations. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 5458-5467	6.4	15
34	ELSI An open infrastructure for electronic structure solvers. <i>Computer Physics Communications</i> , 2020 , 256, 107459	4.2	14
33	Approximate Green's Function Coupled Cluster Method Employing Effective Dimension Reduction. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 3185-3196	6.4	12
32	The parallelization of SPIDER on distributed-memory computers using MPI. <i>Journal of Structural Biology</i> , 2007 , 157, 240-9	3.4	12
31	From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape. <i>Chemical Reviews</i> , 2021 , 121, 4962-4998	68.1	12
30	Optimized Pair Natural Orbitals for the Coupled Cluster Methods. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 4581-4589	6.4	11
29	Model Order Reduction Algorithm for Estimating the Absorption Spectrum. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 4950-4961	6.4	11

28	Numerical integration for ab initio many-electron self energy calculations within the GW approximation. <i>Journal of Computational Physics</i> , 2015 , 286, 1-13	4.1	11
27	Low rank approximation in G 0 W 0 calculations. <i>Science China Mathematics</i> , 2016 , 59, 1593-1612	0.8	10
26	A Structure Preserving Lanczos Algorithm for Computing the Optical Absorption Spectrum. <i>SIAM Journal on Matrix Analysis and Applications</i> , 2018 , 39, 683-711	1.5	10
25	A posteriori 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	9
24	Accelerating Optical Absorption Spectra and Exciton Energy Computation via Interpolative Separable Density Fitting. <i>Lecture Notes in Computer Science</i> , 2018 , 604-617	0.9	9
23	Some remarks on the complex J-symmetric eigenproblem. <i>Linear Algebra and Its Applications</i> , 2018 , 544, 407-442	0.9	9
22	Computing resonant modes of accelerator cavities by solving nonlinear eigenvalue problems via rational approximation. <i>Journal of Computational Physics</i> , 2018 , 374, 1031-1043	4.1	7
21	PSelInv: A distributed memory parallel algorithm for selected inversion: The non-symmetric case. <i>Parallel Computing</i> , 2018 , 74, 84-98	1	6
20	Scalable implementation of polynomial filtering for density functional theory calculation in PARSEC. <i>Computer Physics Communications</i> , 2020 , 254, 107330	4.2	4
19	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	2.8	4
18	Computational simulation of polymer particle structures: vibrational normal modes using the time averaged normal coordinate analysis method. <i>Polymer</i> , 2003 , 44, 3761-3767	3.9	3
17	Normal Coordinate Analysis for Polymer Systems: Capabilities and New Opportunities. <i>Macromolecular Theory and Simulations</i> , 2002 , 11, 711-728	1.5	2
16	An Efficient Algorithm for Calculating the Heat Capacity of a Large-Scale Molecular System. <i>Macromolecular Theory and Simulations</i> , 2001 , 10, 756-761	1.5	2
15	A Scalable Matrix-Free Iterative Eigensolver for Studying Many-Body Localization 2020 ,		2
14	A greedy algorithm for computing eigenvalues of a symmetric matrix with localized eigenvectors. <i>Numerical Linear Algebra With Applications</i> , 2021 , 28, e2341	1.6	2
13	KSSOLV 2.0: An efficient MATLAB toolbox for solving the Kohn-Sham equations with plane-wave basis set. <i>Computer Physics Communications</i> , 2022 , 108424	4.2	2
12	Mesh independence of the generalized Davidson algorithm. <i>Journal of Computational Physics</i> , 2020 , 409, 109322	4.1	1
11	Matrix-free constructions of circulant and block circulant preconditioners. <i>Numerical Linear Algebra With Applications</i> , 2004 , 11, 773-793	1.6	1

10	Large-Scale Normal Coordinate Analysis on Distributed Memory Parallel Systems. <i>International Journal of High Performance Computing Applications</i> , 2002 , 16, 409-424	1.8	1
9	Accelerating an iterative eigensolver for nuclear structure configuration interaction calculations on GPUs using OpenACC. <i>Journal of Computational Science</i> , 2022 , 59, 101554	3.4	1
8	A Shift Selection Strategy for Parallel Shift-invert Spectrum Slicing in Symmetric Self-consistent Eigenvalue Computation. <i>ACM Transactions on Mathematical Software</i> , 2020 , 46, 1-31	2.3	1
7	Quantum Fourier transform revisited. <i>Numerical Linear Algebra With Applications</i> , 2021 , 28,	1.6	1
6	Reinforcement Learning Configuration Interaction. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 5482-5491	6.4	1
5	Computing the density of states for optical spectra of molecules by low-rank and QTT tensor approximation. <i>Journal of Computational Physics</i> , 2019 , 382, 221-239	4.1	
4	Minimizing the Kohn-Sham total energy for periodic systems. <i>Linear Algebra and Its Applications</i> , 2012 , 436, 2764-2779	0.9	
3	Low rank approximation in simulations of quantum algorithms. <i>Journal of Computational Science</i> , 2022 , 59, 101561	3.4	
2	Properties of Definite Bethe-Salpeter Eigenvalue Problems. <i>Lecture Notes in Computational Science and Engineering</i> , 2017 , 91-105	0.3	
1	Accelerating Quantum Many-Body Configuration Interaction with Directives. <i>Lecture Notes in Computer Science</i> , 2022 , 112-132	0.9	