Wei Hu

List of Publications by Year
in descending order

103 papers	4,534 citations	109321 35 h-index	106344 65 g-index
105 all docs	105 docs citations	105 times ranked	4926 citing authors

#	Article	IF	Citations
1	Mixed magnetic edge states in graphene quantum dots. Multifunctional Materials, 2022, 5, 014001.	3.7	1
2	Computational characterization of nanosystems. Chinese Journal of Chemical Physics, 2022, 35, 1-15.	1.3	2
3	High-Throughput Screening of Rattling-Induced Ultralow Lattice Thermal Conductivity in Semiconductors. Journal of the American Chemical Society, 2022, 144, 4448-4456.	13.7	26
4	Low-Rank Approximations Accelerated Plane-Wave Hybrid Functional Calculations with k-Point Sampling. Journal of Chemical Theory and Computation, 2022, 18, 206-218.	5.3	17
5	Designing Direct Z-Scheme Heterojunctions Enabled by Edge-Modified Phosphorene Nanoribbons for Photocatalytic Overall Water Splitting. Journal of Physical Chemistry Letters, 2022, 13, 1-11.	4.6	21
6	KSSOLV 2.0: An efficient MATLAB toolbox for solving the Kohn-Sham equations with plane-wave basis set. Computer Physics Communications, 2022, 279, 108424.	7.5	9
7	Identifying Photocatalytic Active Sites of C₂H₆ Câ€“H Bond Activation on TiO₂ via Combining First-Principles Ground-State and Excited-State Electronic Structure Calculations. Journal of Physical Chemistry Letters, 2022, 13, 6532-6540.	4.6	6
8	High performance computing of DGDFT for tens of thousands of atoms using millions of cores on Sunway TaihuLight. Science Bulletin, 2021, 66, 111-119.	9.0	16
9	Tunable Rashba Spin Splitting in Two-Dimensional Polar Perovskites. Journal of Physical Chemistry Letters, 2021, 12, 1932-1939.	4.6	22
10	Two-level iterative solver for linear response time-dependent density functional theory with plane wave basis set. Journal of Chemical Physics, 2021, 154, 064101.	3.0	10
11	Tuning the Charge Transfer Dynamics of the Nanostructured GaN Photoelectrodes for Efficient Photoelectrochemical Detection in the Ultraviolet Band. Advanced Functional Materials, 2021, 31, 2103007.	14.9	50
12	Hybrid MPI and OpenMP parallel implementation of large-scale linear-response time-dependent density functional theory with plane-wave basis set. Electronic Structure, 2021, 3, 024004.	2.8	4
13	Editorial: Advances in Density Functional Theory and Beyond for Computational Chemistry. Frontiers in Chemistry, 2021, 9, 705762.	3.6	7
14	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.	2.5	13
15	Bidirectional photocurrent in pâ€“n heterojunction nanowires. Nature Electronics, 2021, 4, 645-652.	26.0	129
16	On derived equivalences and homological dimensions. Journal Fur Die Reine Und Angewandte Mathematik, 2021, 2021, 59-85.	0.9	3
17	Two-Dimensional Giant Tunable Rashba Semiconductors with Two-Atom-Thick Buckled Honeycomb Structure. Nano Letters, 2021, 21, 740-746.	9.1	38
18	KSSOLV-GPU: An efficient GPU-enabled MATLAB toolbox for solving the Kohn-Sham equations within density functional theory in plane-wave basis set. Chinese Journal of Chemical Physics, 2021, 34, 552-564.	1.3	9

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19	Designing Two-Dimensional Versatile Room-Temperature Ferromagnets via Assembling Large-Scale Magnetic Quantum Dots. Nano Letters, 2021, 21, 9816-9823.	9.1	11
20	Spinâ€“Orbit Coupling in 2D Semiconductors: A Theoretical Perspective. Journal of Physical Chemistry Letters, 2021, 12, 12256-12268.	4.6	22
21	The static parallel distribution algorithms for hybrid density-functional calculations in HONPAS package. International Journal of High Performance Computing Applications, 2020, 34, 159-168.	3.7	2
22	Approximations, ghosts and derived equivalences. Proceedings of the Royal Society of Edinburgh Section A: Mathematics, 2020, 150, 813-840.	1.2	0
23	Accelerating Excitation Energy Computation in Molecules and Solids within Linear-Response Time-Dependent Density Functional Theory via Interpolative Separable Density Fitting Decomposition. Journal of Chemical Theory and Computation, 2020, 16, 964-973.	5.3	23
24	Machine Learning K-Means Clustering Algorithm for Interpolative Separable Density Fitting to Accelerate Hybrid Functional Calculations with Numerical Atomic Orbitals. Journal of Physical Chemistry A, 2020, 124, 10066-10074.	2.5	35
25	Highly efficient heterojunction solar cells enabled by edge-modified tellurene nanoribbons. Physical Chemistry Chemical Physics, 2020, 22, 28414-28422.	2.8	8
26	Hydrogenâ€Dopingâ€Induced Metalâ€Like Ultrahigh Freeâ€Carrier Concentration in Metalâ€Oxide Material for Giant and Tunable Plasmon Resonance. Advanced Materials, 2020, 32, e2004059.	21.0	57
27	A Machine Learning Protocol for Predicting Protein Infrared Spectra. Journal of the American Chemical Society, 2020, 142, 19071-19077.	13.7	55
28	Photogenerated-Carrier Separation and Transfer in Two-Dimensional Janus Transition Metal Dichalcogenides and Graphene van der Waals Sandwich Heterojunction Photovoltaic Cells. Journal of Physical Chemistry Letters, 2020, 11, 4070-4079.	4.6	44
29	Tunable n-type and p-type doping of two-dimensional layered PdSe₂via organic molecular adsorption. Physical Chemistry Chemical Physics, 2020, 22, 12973-12979.	2.8	15
30	Interpolative Separable Density Fitting Decomposition for Accelerating Hartreeâ€“Fock Exchange Calculations within Numerical Atomic Orbitals. Journal of Physical Chemistry A, 2020, 124, 5664-5674.	2.5	18
31	Two-dimensional Ca4N2 as a one-dimensional electride [Ca4N2]2+Â·2eâ€™ with ultrahigh conductance. Nanoscale, 2020, 12, 5578-5586.	5.6	3
32	Tunable Rashba spin splitting in Janus transition-metal dichalcogenide monolayers via charge doping. RSC Advances, 2020, 10, 6388-6394.	3.6	55
33	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, .	3.2	14
34	Parallel Implementation of Large-Scale Linear Scaling Density Functional Theory Calculations With Numerical Atomic Orbitals in HONPAS. Frontiers in Chemistry, 2020, 8, 589910.	3.6	2
35	Gorenstein projective bimodules via monomorphism categories and filtration categories. Journal of Pure and Applied Algebra, 2019, 223, 1014-1039.	0.6	8
36	Tunable Schottky and Ohmic contacts in graphene and tellurene van der Waals heterostructures. Physical Chemistry Chemical Physics, 2019, 21, 23611-23619.	2.8	24

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37	First-principles study of Pd single-atom catalysis to hydrogen desorption reactions on MgH2(110) surface. Chinese Journal of Chemical Physics, 2019, 32, 319-326.	1.3	3
38	Bifacial Raman Enhancement on Monolayer Two-Dimensional Materials. Nano Letters, 2019, 19, 1124-1130.	9.1	10
39	Room-temperature magnetism and tunable energy gaps in edge-passivated zigzag graphene quantum dots. Npj 2D Materials and Applications, 2019, 3, .	7.9	25
40	Highly-efficient heterojunction solar cells based on two-dimensional tellurene and transition metal dichalcogenides. Journal of Materials Chemistry A, 2019, 7, 7430-7436.	10.3	90
41	Control of highly anisotropic electrical conductance of tellurene by strain-engineering. Nanoscale, 2019, 11, 21775-21781.	5.6	11
42	Metal-Free Boron Nitride Nanoribbon Catalysts for Electrochemical CO₂ Reduction: Combining High Activity and Selectivity. ACS Applied Materials & Interfaces, 2019, 11, 906-915.	8.0	66
43	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.	5.3	39
44	Doped phosphorene for hydrogen capture: A DFT study. Applied Surface Science, 2018, 433, 249-255.	6.1	48
45	Intrinsic Electric Fields in Two-dimensional Materials Boost the Solar-to-Hydrogen Efficiency for Photocatalytic Water Splitting. Nano Letters, 2018, 18, 6312-6317.	9.1	391
46	Derived equivalences and stable equivalences of Morita type, II. Revista Matematica Iberoamericana, 2018, 34, 59-110.	0.9	7
47	Theoretical Design of a Two-Photon Fluorescent Probe for Nitric Oxide with Enhanced Emission Induced by Photoninduced Electron Transfer. Sensors, 2018, 18, 1324.	3.8	14
48	Monitoring Reaction Paths Using Vibrational Spectroscopies: The Case of the Dehydrogenation of Propane toward Propylene on Pd-Doped Cu(111) Surface. Molecules, 2018, 23, 126.	3.8	7
49	Accelerating Optical Absorption Spectra and Exciton Energy Computation via Interpolative Separable Density Fitting. Lecture Notes in Computer Science, 2018, , 604-617.	1.3	12
50	Visualizing subsurface defects in graphite by acoustic atomic force microscopy. Microscopy Research and Technique, 2017, 80, 66-74.	2.2	12
51	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.	5.3	38
52	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.	3.8	29
53	Effects of line defects on the electronic properties of ZnO nanoribbons and sheets. Journal of Materials Chemistry C, 2017, 5, 3121-3129.	5.5	16
54	Thermionic Energy Conversion Based on Graphene van der Waals Heterostructures. Scientific Reports, 2017, 7, 46211.	3.3	53

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55	Stable functors of derived equivalences and Gorenstein projective modules. Mathematische Nachrichten, 2017, 290, 1512-1530.	0.8	8
56	Water on silicene: A hydrogen bond-autocatalyzed physisorptionâ€“chemisorptionâ€“dissociation transition. Nano Research, 2017, 10, 2223-2233.	10.4	21
57	[Ti₁₂In₆O₁₈(OOCC₆H₅)₃₀]: a multifunctional hetero-polyoxotitanate nanocluster with high stability and visible photoactivity. Dalton Transactions, 2017, 46, 678-684.	3.3	31
58	Highly Efficient Photocatalytic Water Splitting over Edge-Modified Phosphorene Nanoribbons. Journal of the American Chemical Society, 2017, 139, 15429-15436.	13.7	244
59	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.	5.3	53
60	Projected Commutator DIIS Method for Accelerating Hybrid Functional Electronic Structure Calculations. Journal of Chemical Theory and Computation, 2017, 13, 5458-5467.	5.3	21
61	Stable Heteropolyoxotitanate Nanocluster for Full Solar Spectrum Photocatalytic Hydrogen Evolution. Journal of Physical Chemistry C, 2017, 121, 18326-18332.	3.1	20
62	Two-dimensional van der Waals heterojunctions for functional materials and devices. Journal of Materials Chemistry C, 2017, 5, 12289-12297.	5.5	151
63	Identifying the structure of 4-chlorophenyl isocyanide adsorbed on Au(111) and Pt(111) surfaces by first-principles simulations of Raman spectra. Physical Chemistry Chemical Physics, 2017, 19, 32389-32397.	2.8	12
64	Conjugation Length Effect on TPA-Based Optical Limiting Performance of a Series of Ladder-Type Chromophores. Materials, 2017, 10, 70.	2.9	2
65	Energy Donor Effect on the Sensing Performance for a Series of FRET-Based Two-Photon Fluorescent Hg2+ Probes. Materials, 2017, 10, 108.	2.9	6
66	Chebyshev polynomial filtered subspace iteration in the discontinuous Galerkin method for large-scale electronic structure calculations. Journal of Chemical Physics, 2016, 145, 154101.	3.0	28
67	A modified Schottky model for graphene-semiconductor (3D/2D) contact: A combined theoretical and experimental study. , 2016, , .		19
68	Systematic Synthesis of Tellurium Nanostructures and Their Optical Properties: From Nanoparticles to Nanorods, Nanowires, and Nanotubes. ChemNanoMat, 2016, 2, 167-170.	2.8	61
69	Edge-Modified Phosphorene Nanoflake Heterojunctions as Highly Efficient Solar Cells. Nano Letters, 2016, 16, 1675-1682.	9.1	176
70	Effects of interlayer coupling and electric fields on the electronic structures of graphene and MoS₂heterobilayers. Journal of Materials Chemistry C, 2016, 4, 1776-1781.	5.5	114
71	First-principles study of two-dimensional van der Waals heterojunctions. Computational Materials Science, 2016, 112, 518-526.	3.0	88
72	DGDFT: A massively parallel method for large scale density functional theory calculations. Journal of Chemical Physics, 2015, 143, 124110.	3.0	55

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73	Molecular Design to Enhance the Thermal Stability of a Photo Switchable Molecular Junction Based on Dimethyldihydropyrene and Cyclophanediene Isomerization. Journal of Physical Chemistry C, 2015, 119, 11468-11474.	3.1	14
74	Edge reconstruction in armchair phosphorene nanoribbons revealed by discontinuous Galerkin density functional theory. Physical Chemistry Chemical Physics, 2015, 17, 31397-31404.	2.8	37
75	Large birefringence smectic-A liquid crystals for high contrast bistable displays. Optical Materials Express, 2015, 5, 281.	3.0	8
76	Tunable Schottky contacts in hybrid grapheneâ€“phosphorene nanocomposites. Journal of Materials Chemistry C, 2015, 3, 4756-4761.	5.5	116
77	Defects in Phosphorene. Journal of Physical Chemistry C, 2015, 119, 20474-20480.	3.1	215
78	Quasi-Analytical Approach for Modeling of Surface-Enhanced Raman Scattering. Journal of Physical Chemistry C, 2015, 119, 28992-28998.	3.1	13
79	Electronic structure and aromaticity of large-scale hexagonal graphene nanoflakes. Journal of Chemical Physics, 2014, 141, 214704.	3.0	40
80	Silicene as a highly sensitive molecule sensor for NH3, NO and NO2. Physical Chemistry Chemical Physics, 2014, 16, 6957.	2.8	221
81	A first-principles study of gas adsorption on germanene. Physical Chemistry Chemical Physics, 2014, 16, 22495-22498.	2.8	232
82	Feasible Catalytic Strategy for Writing Conductive Nanoribbons on a Single-Layer Graphene Fluoride. Journal of Physical Chemistry C, 2014, 118, 22643-22648.	3.1	0
83	Semiconductor Alloy Nanoribbon Lateral Heterostructures for Highâ€Performance Photodetectors. Advanced Materials, 2014, 26, 2844-2849.	21.0	70
84	Helium separation via porous silicene based ultimate membrane. Nanoscale, 2013, 5, 9062.	5.6	96
85	Structural, electronic, and optical properties of hybrid silicene and graphene nanocomposite. Journal of Chemical Physics, 2013, 139, 154704.	3.0	84
86	Surface and size effects on the charge state of NV center in nanodiamonds. Computational and Theoretical Chemistry, 2013, 1021, 49-53.	2.5	17
87	Porous silicene as a hydrogen purification membrane. Physical Chemistry Chemical Physics, 2013, 15, 5753.	2.8	127
88	Nondecaying long range effect of surface decoration on the charge state of NV center in diamond. Journal of Chemical Physics, 2013, 138, 034702.	3.0	6
89	Electronic and optical properties of graphene and graphitic ZnO nanocomposite structures. Journal of Chemical Physics, 2013, 138, 124706.	3.0	97
90	Pressure Sensors: A Flexible and Highly Pressure-Sensitive Graphene-Polyurethane Sponge Based on Fractured Microstructure Design (Adv. Mater. 46/2013). Advanced Materials, 2013, 25, 6691-6691.	21.0	17

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91	Diamond as an inert substrate of graphene. Journal of Chemical Physics, 2013, 138, 054701.	3.0	46
92	Derived equivalences for Î¦-Auslander-Yoneda algebras. Transactions of the American Mathematical Society, 2013, 365, 5681-5711.	0.9	17
93	Derived equivalences from cohomological approximations and mutations of Î¦-Yoneda algebras. Proceedings of the Royal Society of Edinburgh Section A: Mathematics, 2013, 143, 589-629.	1.2	9
94	Bistable state in polymer stabilized blue phase liquid crystal. Optical Materials Express, 2012, 2, 1353.	3.0	5
95	Large birefringence liquid crystal material in terahertz range. Optical Materials Express, 2012, 2, 1314.	3.0	104
96	On Iterated Almost Î½-Stable Derived Equivalences. Communications in Algebra, 2012, 40, 3920-3932.	0.6	2
97	Half-Metallicity in Organic Single Porous Sheets. Journal of the American Chemical Society, 2012, 134, 5718-5721.	13.7	101
98	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mi mathvariant="script">D</mml:mi></mml:math>-split sequences and derived equivalences. Advances in Mathematics, 2011, 227, 292-318.	1.1	33
99	Derived equivalences and stable equivalences of Morita type, I. Nagoya Mathematical Journal, 2010, 200, 107-152.	0.8	33
100	Tilting modules and representation dimensions. Journal of Algebra, 2010, 323, 738-748.	0.7	3
101	Derived equivalences and stable equivalences of Morita type, I. Nagoya Mathematical Journal, 2010, 200, 107-152.	0.8	6
102	Auslander-Reiten sequences and global dimensions. Mathematical Research Letters, 2006, 13, 885-895.	0.5	5
103	Dominant and global dimension of blocks of quantised Schur algebras. Mathematische Zeitschrift, 0, , 1.	0.9	0