

Xu Zhang

List of Publications by Year in descending order

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122
papers

10,117
citations

109264

35
h-index

34964

98
g-index

125
all docs

125
docs citations

125
times ranked

12609
citing authors

#	ARTICLE	IF	CITATIONS
1	CoNi nano-alloy anchored on biomass-derived N-doped carbon frameworks for enhanced oxygen reduction and evolution reactions. <i>Electrochimica Acta</i> , 2022, 402, 139555.	2.6	17
2	Controlling Localized Plasmons via an Atomistic Approach: Attainment of Site-Selective Activation inside a Single Molecule. <i>Journal of the American Chemical Society</i> , 2022, 144, 2051-2055.	6.6	14
3	Understanding Quantum Plasmonic Enhancement in Nanorod Dimers from Time-Dependent Orbital-Free Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2022, 126, 5046-5054.	1.5	3
4	Chemically identifying single adatoms with single-bond sensitivity during oxidation reactions of borophene. <i>Nature Communications</i> , 2022, 13, 1796.	5.8	18
5	Microengineered Multi-Organoid System from hiPSCs to Recapitulate Human Liver Islet Axis in Normal and Type 2 Diabetes. <i>Advanced Science</i> , 2022, 9, e2103495.	5.6	49
6	HiPSC-derived multi-organoids-on-chip system for safety assessment of antidepressant drugs. <i>Lab on A Chip</i> , 2021, 21, 571-581.	3.1	56
7	A flexible microfluidic strategy to generate grooved microfibers for guiding cell alignment. <i>Biomaterials Science</i> , 2021, 9, 4880-4890.	2.6	23
8	Frenkel defects promote polaronic exciton dissociation in methylammonium lead iodide perovskites. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 6583-6590.	1.3	2
9	Simple and fast isolation of circulating exosomes with a chitosan modified shuttle flow microchip for breast cancer diagnosis. <i>Lab on A Chip</i> , 2021, 21, 1759-1770.	3.1	33
10	A hierarchically ordered porous nitrogen-doped carbon catalyst with densely accessible Co-N active sites for efficient oxygen reduction reaction. <i>Microporous and Mesoporous Materials</i> , 2021, 317, 111002.	2.2	12
11	SARS-CoV-2 induced intestinal responses with a biomimetic human gut-on-chip. <i>Science Bulletin</i> , 2021, 66, 783-793.	4.3	91
12	Data driven discovery of conjugated polyelectrolytes for optoelectronic and photocatalytic applications. <i>Npj Computational Materials</i> , 2021, 7, .	3.5	19
13	Moiré excitons in defective van der Waals heterostructures. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	3.3	16
14	Angstrom-Scale Spectroscopic Visualization of Interfacial Interactions in an Organic/Borophene Vertical Heterostructure. <i>Journal of the American Chemical Society</i> , 2021, 143, 15624-15634.	6.6	29
15	One-Dimensional Flat Bands and Anisotropic Moiré Excitons in Twisted Tin Sulfide Bilayers. <i>Chemistry of Materials</i> , 2021, 33, 7432-7440.	3.2	6
16	Predictions of moiré excitons in twisted two-dimensional organic-inorganic halide perovskites. <i>Chemical Science</i> , 2021, 12, 6073-6080.	3.7	5
17	Unraveling Structural and Optical Properties of Two-Dimensional $\text{Mo}_x\text{W}_{1-x}\text{S}_2$ Alloys. <i>Journal of Physical Chemistry C</i> , 2021, 125, 774-781.	1.5	17
18	Unraveling energy and charge transfer in type-II van der Waals heterostructures. <i>Npj Computational Materials</i> , 2021, 7, .	3.5	16

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19	Unveiling the Nature of Light-Triggered Hole Traps in Lead Halide Perovskites: A Study with Time-Dependent Density Functional Theory. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 12075-12083.	2.1	3
20	Defining Multiple Configurations of Rubrene on a Ag(100) Surface with 5 Å... Spatial Resolution via Ultrahigh Vacuum Tip-Enhanced Raman Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2020, 124, 2420-2426.	1.5	26
21	Linear-Response Time-Dependent Density Functional Theory with Stochastic Range-Separated Hybrids. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 1064-1072.	2.3	19
22	Quantum Plasmonics in Nanorods: A Time-Dependent Orbital-Free Density Functional Theory Study with Thousands of Atoms. <i>Journal of Physical Chemistry C</i> , 2020, 124, 945-951.	1.5	13
23	Charge separation boosts exciton diffusion in fused ring electron acceptors. <i>Journal of Materials Chemistry A</i> , 2020, 8, 23304-23312.	5.2	18
24	Shedding light on moiré excitons: A first-principles perspective. <i>Science Advances</i> , 2020, 6, .	4.7	50
25	Intramolecular Band Alignment and Spin-Orbit Coupling in Two-Dimensional Halide Perovskites. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 6982-6989.	2.1	24
26	Excitonic Effect Drives Ultrafast Dynamics in van der Waals Heterostructures. <i>Nano Letters</i> , 2020, 20, 4631-4637.	4.5	46
27	AgPd nanoparticles for electrocatalytic CO ₂ reduction: bimetallic composition-dependent ligand and ensemble effects. <i>Nanoscale</i> , 2020, 12, 14068-14075.	2.8	36
28	Band Alignment in Two-Dimensional Halide Perovskite Heterostructures: Type I or Type II?. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 2910-2916.	2.1	43
29	Organic Cations Protect Methylammonium Lead Iodide Perovskites against Small Exciton-Polaron Formation. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 2983-2991.	2.1	12
30	Impact of ball-milling and ionic liquid pretreatments on pyrolysis kinetics and behaviors of crystalline cellulose. <i>Bioresource Technology</i> , 2020, 305, 123044.	4.8	31
31	Reducing Anomalous Hysteresis in Perovskite Solar Cells by Suppressing the Interfacial Ferroelectric Order. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 12275-12284.	4.0	13
32	Zn ⁺ O ⁻ Dual-Spin Surface State Formation by Modification of ZnO Nanoparticles with Diboron Compounds. <i>Langmuir</i> , 2019, 35, 14173-14179.	1.6	5
33	Unraveling photoexcitation dynamics at in-a-perovskite-heterojunctions from first-principles. <i>Journal of Materials Chemistry A</i> , 2019, 7, 18012-18019.	5.2	12
34	In Situ Self-Assembly of Ultrastable Gold Nanoparticles on Polyvinyl Alcohol Nanofibrous Mats for Use as Highly Reusable Catalysts. <i>ACS Omega</i> , 2019, 4, 20094-20100.	1.6	3
35	Generalized Synthetic Strategy for Transition-Metal-Doped Brookite-Phase TiO ₂ Nanorods. <i>Journal of the American Chemical Society</i> , 2019, 141, 16548-16552.	6.6	78
36	Modification of TiO ₂ Nanoparticles with Organodiboron Molecules Inducing Stable Surface Ti ³⁺ Complex. <i>IScience</i> , 2019, 20, 195-204.	1.9	24

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37	PdMo bimetallic for oxygen reduction catalysis. <i>Nature</i> , 2019, 574, 81-85.	13.7	935
38	Radiative recombination of large polarons in halide perovskites. <i>Journal of Physics Condensed Matter</i> , 2019, 31, 165701.	0.7	5
39	Decreasing Exciton Binding Energy in Two-Dimensional Halide Perovskites by Lead Vacancies. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 3820-3827.	2.1	27
40	Self-Healing of Photocurrent Degradation in Perovskite Solar Cells: The Role of Defect-Trapped Excitons. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 7774-7780.	2.1	23
41	Phase Transition Control for High Performance Ruddlesden-Popper Perovskite Solar Cells. <i>Advanced Materials</i> , 2018, 30, e1707166.	11.1	244
42	Coupled quantum mechanics/molecular mechanics modeling of metallic materials: Theory and applications. <i>Journal of Materials Research</i> , 2018, 33, 796-812.	1.2	4
43	How Methylammonium Cations and Chlorine Dopants Heal Defects in Lead Iodide Perovskites. <i>Advanced Energy Materials</i> , 2018, 8, 1702754.	10.2	86
44	Stable High-Index Faceted Pt Skin on Zigzag-Like Pt/Fe Nanowires Enhances Oxygen Reduction Catalysis. <i>Advanced Materials</i> , 2018, 30, 1705515.	11.1	305
45	Stable High-Performance Perovskite Solar Cells via Grain Boundary Passivation. <i>Advanced Materials</i> , 2018, 30, e1706576.	11.1	665
46	Macro-micron-nano-featured surface topography of Ti-6Al-4V alloy for biomedical applications. <i>Rare Metals</i> , 2018, 37, 1055-1063.	3.6	26
47	Favorable Core/Shell Interface within Co ₂ P/Pt Nanorods for Oxygen Reduction Electrocatalysis. <i>Nano Letters</i> , 2018, 18, 7870-7875.	4.5	68
48	First-order nonadiabatic couplings in extended systems by time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2018, 149, 244103.	1.2	8
49	Multi-inch single-crystalline perovskite membrane for high-detectivity flexible photosensors. <i>Nature Communications</i> , 2018, 9, 5302.	5.8	212
50	Healing detrimental defects in two-dimensional semiconductors through strain engineering. <i>Semiconductor Science and Technology</i> , 2018, 33, 075005.	1.0	0
51	A 1300 mm ² Ultrahigh-Performance Digital Imaging Assembly using High-Quality Perovskite Single Crystals. <i>Advanced Materials</i> , 2018, 30, e1707314.	11.1	246
52	Large-scale ab initio calculations of Raman scattering spectra within time-dependent density functional perturbation theory. <i>Journal of Chemical Physics</i> , 2018, 148, 244103.	1.2	5
53	Ultrathin PtPd-Based Nanorings with Abundant Step Atoms Enhance Oxygen Catalysis. <i>Advanced Materials</i> , 2018, 30, e1802136.	11.1	107
54	Optically inactive defects in monolayer and bilayer phosphorene: A first-principles study. <i>Physical Review Materials</i> , 2018, 2, .	0.9	21

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55	Multiscale Computational Design of Core/Shell Nanoparticles for Oxygen Reduction Reaction. <i>Journal of Physical Chemistry C</i> , 2017, 121, 1964-1973.	1.5	27
56	Probing the Bi-directional Interaction Between Microglia and Gliomas in a Tumor Microenvironment on a Microdevice. <i>Neurochemical Research</i> , 2017, 42, 1478-1487.	1.6	12
57	Precise tuning in platinum-nickel/nickel sulfide interface nanowires for synergistic hydrogen evolution catalysis. <i>Nature Communications</i> , 2017, 8, 14580.	5.8	648
58	Efficient oxygen reduction catalysis by subnanometer Pt alloy nanowires. <i>Science Advances</i> , 2017, 3, e1601705.	4.7	330
59	Plasmonic resonances of nanoparticles from large-scale quantum mechanical simulations. <i>International Journal of Modern Physics B</i> , 2017, 31, 1740003.	1.0	5
60	Effect of Point Defects on Optical Properties of Graphene Fluoride: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2017, 121, 12855-12862.	1.5	30
61	Stable high efficiency two-dimensional perovskite solar cells via cesium doping. <i>Energy and Environmental Science</i> , 2017, 10, 2095-2102.	15.6	588
62	Charge transport in hybrid halide perovskites. <i>Physical Review B</i> , 2017, 96, .	1.1	22
63	Comment on "Linear Scaling of the Exciton Binding Energy versus the Band Gap of Two-Dimensional Materials". <i>Physical Review Letters</i> , 2017, 118, 209701.	2.9	8
64	Ordered PdCu-Based Nanoparticles as Bifunctional Oxygen-Reduction and Ethanol-Oxidation Electrocatalysts. <i>Angewandte Chemie</i> , 2016, 128, 9176-9181.	1.6	56
65	Ordered PdCu-Based Nanoparticles as Bifunctional Oxygen-Reduction and Ethanol-Oxidation Electrocatalysts. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 9030-9035.	7.2	278
66	Quantum electrodynamics and plasmonic resonance of metallic nanostructures. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 155302.	0.7	2
67	Biaxially strained PtPb/Pt core/shell nanoplate boosts oxygen reduction catalysis. <i>Science</i> , 2016, 354, 1410-1414.	6.0	1,262
68	Charge Stripe Formation in Molecular Ferroelectric Organohalide Perovskites for Efficient Charge Separation. <i>Journal of Physical Chemistry C</i> , 2016, 120, 23969-23975.	1.5	14
69	Generalized Surface Coordination Number as an Activity Descriptor for CO ₂ Reduction on Cu Surfaces. <i>Journal of Physical Chemistry C</i> , 2016, 120, 28125-28130.	1.5	77
70	Surface engineering of hierarchical platinum-cobalt nanowires for efficient electrocatalysis. <i>Nature Communications</i> , 2016, 7, 11850.	5.8	607
71	The lowest-energy charge-transfer state and its role in charge separation in organic photovoltaics. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 17546-17556.	1.3	17
72	Understanding Quantum Plasmonics from Time-Dependent Orbital-Free Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2016, 120, 14330-14336.	1.5	29

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73	Patterning hypoxic multicellular spheroids in a 3D matrix – a promising method for anti-tumor drug screening. <i>Biotechnology Journal</i> , 2016, 11, 127-134.	1.8	20
74	Subspace formulation of time-dependent density functional theory for large-scale calculations. <i>Journal of Chemical Physics</i> , 2015, 143, 064110.	1.2	24
75	A General Method for Multimetallic Platinum Alloy Nanowires as Highly Active and Stable Oxygen Reduction Catalysts. <i>Advanced Materials</i> , 2015, 27, 7204-7212.	11.1	280
76	Activation of hypoxia signaling induces phenotypic transformation of glioma cells: implications for bevacizumab antiangiogenic therapy. <i>Oncotarget</i> , 2015, 6, 11882-11893.	0.8	68
77	Microdevices: Flexible Fabrication of Shape-Controlled Collagen Building Blocks for Self-Assembly of 3D Microtissues (<i>Small</i> 30/2015). <i>Small</i> , 2015, 11, 3665-3665.	5.2	2
78	Chemical tuning of band alignments for Cu/HfO ₂ interfaces. <i>Physica Status Solidi (B): Basic Research</i> , 2015, 252, 298-304.	0.7	3
79	Do “Hot” Charge-Transfer Excitons Promote Free Carrier Generation in Organic Photovoltaics?. <i>Journal of Physical Chemistry C</i> , 2015, 119, 15028-15035.	1.5	27
80	Flexible Fabrication of Shape-Controlled Collagen Building Blocks for Self-Assembly of 3D Microtissues. <i>Small</i> , 2015, 11, 3666-3675.	5.2	24
81	A New Core/Shell NiAu/Au Nanoparticle Catalyst with Pt-like Activity for Hydrogen Evolution Reaction. <i>Journal of the American Chemical Society</i> , 2015, 137, 5859-5862.	6.6	274
82	Core/Shell Face-Centered Tetragonal FePd/Pd Nanoparticles as an Efficient Non-Pt Catalyst for the Oxygen Reduction Reaction. <i>ACS Nano</i> , 2015, 9, 11014-11022.	7.3	165
83	Overpotential for CO ₂ electroreduction lowered on strained penta-twinned Cu nanowires. <i>Chemical Science</i> , 2015, 6, 6829-6835.	3.7	60
84	Strongly Interacting C ₆₀ /Ir(111) Interface: Transformation of C ₆₀ into Graphene and Influence of Graphene Interlayer. <i>Journal of Physical Chemistry C</i> , 2015, 119, 27550-27555.	1.5	13
85	Effects of oxygen on prismatic faults in $\hat{\pm}$ -Ti: a combined quantum mechanics/molecular mechanics study. <i>Scripta Materialia</i> , 2015, 98, 32-35.	2.6	21
86	Understanding molecular structure dependence of exciton diffusion in conjugated small molecules. <i>Applied Physics Letters</i> , 2014, 104, 143303.	1.5	7
87	Helium bubble nucleation and growth in $\hat{\pm}$ -Fe: insights from first-principles simulations. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 255401.	0.7	14
88	Computational Design of Core/Shell Nanoparticles for Oxygen Reduction Reactions. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 292-297.	2.1	71
89	Charge Separation and Exciton Dynamics at Polymer/ZnO Interface from First-Principles Simulations. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 2649-2656.	2.1	48
90	Size-Dependent Plasmonic Resonances from Large-Scale Quantum Simulations. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 1163-1169.	2.1	41

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91	Nanocatalyst Superior to Pt for Oxygen Reduction Reactions: The Case of Core/Shell Ag(Au)/CuPd Nanoparticles. <i>Journal of the American Chemical Society</i> , 2014, 136, 15026-15033.	6.6	172
92	Exciton diffusion in disordered small molecules for organic photovoltaics: insights from first-principles simulations. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 185006.	0.7	8
93	Tuning Nanoparticle Structure and Surface Strain for Catalysis Optimization. <i>Journal of the American Chemical Society</i> , 2014, 136, 7734-7739.	6.6	349
94	Hole Transport in Diketopyrrolopyrrole (DPP) Small Molecules: A Joint Theoretical and Experimental Study. <i>Journal of Physical Chemistry C</i> , 2013, 117, 6730-6740.	1.5	21
95	Atomistic study of plastic deformation in Mg-Al alloys. <i>Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2013, 586, 245-252.	2.6	30
96	How Cr changes the dislocation core structure of α -Fe: the role of magnetism. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 085403.	0.7	1
97	Multiscale quantum/atomistic coupling using constrained density functional theory. <i>Physical Review B</i> , 2013, 87, .	1.1	32
98	A non-self-consistent range-separated time-dependent density functional approach for large-scale simulations. <i>Journal of Physics Condensed Matter</i> , 2012, 24, 205801.	0.7	20
99	First-Principles Study of Electron Mobility in Cationic and Anionic Conjugated Polyelectrolytes. <i>Journal of Physical Chemistry C</i> , 2012, 116, 1205-1210.	1.5	8
100	Flexible Generation of Gradient Electrospinning Nanofibers Using a Microfluidic Assisted Approach. <i>Langmuir</i> , 2012, 28, 10026-10032.	1.6	53
101	Dipole-Assisted Charge Separation in Organic-Inorganic Hybrid Photovoltaic Heterojunctions: Insight from First-Principles Simulations. <i>Journal of Physical Chemistry C</i> , 2012, 116, 9845-9851.	1.5	25
102	First-principles simulations of exciton diffusion in organic semiconductors. <i>Physical Review B</i> , 2011, 84, .	1.1	58
103	A Fortran program for calculating electron or hole mobility in disordered semiconductors from first-principles. <i>Computer Physics Communications</i> , 2011, 182, 2632-2637.	3.0	6
104	Dynamic kinetic energy potential for orbital-free density functional theory. <i>Journal of Chemical Physics</i> , 2011, 134, 144101.	1.2	27
105	Electron structure and dynamics at poly(3-hexylthiophene)/fullerene photovoltaic heterojunctions. <i>Applied Physics Letters</i> , 2011, 98, 083303.	1.5	12
106	Recent Development in Quantum Mechanics/Molecular Mechanics Modeling for Materials. <i>International Journal for Multiscale Computational Engineering</i> , 2011, , .	0.8	1
107	Quantum mechanical study of solid solution effects on dislocation nucleation during nanoindentation. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2010, 18, 075003.	0.8	10
108	Structure, mechanical and thermodynamic stability of vacancy clusters in Cu. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2010, 18, 055009.	0.8	10

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109	Electron Dynamics in Dye-Sensitized Solar Cells: Effects of Surface Terminations and Defects. Journal of Physical Chemistry B, 2010, 114, 17077-17083.	1.2	28
110	Calculation of fast pipe diffusion along a dislocation stacking fault ribbon. Physical Review B, 2010, 82, .	1.1	19
111	Quantum mechanical simulations of nanoindentation of Al thin film. Computational Materials Science, 2010, 47, 769-774.	1.4	10
112	First-principles determination of charge carrier mobility in disordered semiconducting polymers. Physical Review B, 2010, 82, .	1.1	26
113	Self-consistent embedding quantum mechanics/molecular mechanics method with applications to metals. Physical Review B, 2010, 82, .	1.1	15
114	First-principles study of vacancy formation and migration in clean and Re-doped $\text{Fe-Ni}_3\text{Al}$. Acta Materialia, 2009, 57, 224-231.	3.8	27
115	Application of a hybrid quantum mechanics and empirical molecular dynamics multiscale method to carbon nanotubes. European Physical Journal B, 2008, 65, 515-523.	0.6	3
116	Transport properties of an armchair carbon nanotube with a double vacancy under stretching. Journal of Physics Condensed Matter, 2008, 20, 345225.	0.7	2
117	Electronic origin of void formation in fcc metals. Physical Review B, 2008, 77, .	1.1	17
118	First-principles study for transport properties of armchair carbon nanotubes with a double vacancy under strain. Journal of Applied Physics, 2008, 103, 113714.	1.1	5
119	Quantum simulation of materials at micron scales and beyond. Physical Review B, 2008, 78, .	1.1	33
120	Electronic structure analysis of self-consistent embedding theory for quantum/molecular mechanics simulations. Physical Review B, 2008, 78, .	1.1	14
121	Quantum mechanics/molecular mechanics methodology for metals based on orbital-free density functional theory. Physical Review B, 2007, 76, .	1.1	26
122	Chemical Characterization of a Three-Dimensional Double-Decker Molecule on a Surface via Scanning-Tunneling-Microscopy-Based Tip-Enhanced Raman Spectroscopy. Journal of Physical Chemistry C, 0, , .	1.5	4