Xu Zhang

List of Publications by Year
in descending order

122 papers	10,117 citations	109321 35 h-index	33894 99 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. Electrochimica Acta, 2022, 402, 139555.	5.2	17
2	Controlling Localized Plasmons via an Atomistic Approach: Attainment of Site-Selective Activation inside a Single Molecule. Journal of the American Chemical Society, 2022, 144, 2051-2055.	13.7	14
3	Understanding Quantum Plasmonic Enhancement in Nanorod Dimers from Time-Dependent Orbital-Free Density Functional Theory. Journal of Physical Chemistry C, 2022, 126, 5046-5054.	3.1	3
4	Chemically identifying single adatoms with single-bond sensitivity during oxidation reactions of borophene. Nature Communications, 2022, 13, 1796.	12.8	18
5	Microengineered Multiâ€Organoid System from hiPSCs to Recapitulate Human Liverâ€Islet Axis in Normal and Type 2 Diabetes. Advanced Science, 2022, 9, e2103495.	11.2	49
6	HiPSC-derived multi-organoids-on-chip system for safety assessment of antidepressant drugs. Lab on A Chip, 2021, 21, 571-581.	6.0	56
7	A flexible microfluidic strategy to generate grooved microfibers for guiding cell alignment. Biomaterials Science, 2021, 9, 4880-4890.	5.4	23
8	Frenkel defects promote polaronic exciton dissociation in methylammonium lead iodide perovskites. Physical Chemistry Chemical Physics, 2021, 23, 6583-6590.	2.8	2
9	Simple and fast isolation of circulating exosomes with a chitosan modified shuttle flow microchip for breast cancer diagnosis. Lab on A Chip, 2021, 21, 1759-1770.	6.0	33
10	A hierarchically ordered porous nitrogen-doped carbon catalyst with densely accessible Co-N active sites for efficient oxygen reduction reaction. Microporous and Mesoporous Materials, 2021, 317, 111002.	4.4	12
11	SARS-CoV-2 induced intestinal responses with a biomimetic human gut-on-chip. Science Bulletin, 2021, 66, 783-793.	9.0	91
12	Data driven discovery of conjugated polyelectrolytes for optoelectronic and photocatalytic applications. Npj Computational Materials, 2021, 7, .	8.7	19
13	MoirÃ© excitons in defective van der Waals heterostructures. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	16
14	Angstrom-Scale Spectroscopic Visualization of Interfacial Interactions in an Organic/Borophene Vertical Heterostructure. Journal of the American Chemical Society, 2021, 143, 15624-15634.	13.7	29
15	One-Dimensional Flat Bands and Anisotropic MoirÃ© Excitons in Twisted Tin Sulfide Bilayers. Chemistry of Materials, 2021, 33, 7432-7440.	6.7	6
16	Predictions of moirÃ© excitons in twisted two-dimensional organicâ€“inorganic halide perovskites. Chemical Science, 2021, 12, 6073-6080.	7.4	5
17	Unraveling Structural and Optical Properties of Two-Dimensional Mo_xW_{1â€“x}S₂ Alloys. Journal of Physical Chemistry C, 2021, 125, 774-781.	3.1	17
18	Unraveling energy and charge transfer in type-II van der Waals heterostructures. Npj Computational Materials, 2021, 7, .	8.7	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. Journal of Physical Chemistry Letters, 2021, 12, 12075-12083.	4.6	3
20	Defining Multiple Configurations of Rubrene on a Ag(100) Surface with 5 Ã… Spatial Resolution via Ultrahigh Vacuum Tip-Enhanced Raman Spectroscopy. Journal of Physical Chemistry C, 2020, 124, 2420-2426.	3.1	26
21	Linear-Response Time-Dependent Density Functional Theory with Stochastic Range-Separated Hybrids. Journal of Chemical Theory and Computation, 2020, 16, 1064-1072.	5.3	19
22	Quantum Plasmonics in Nanorods: A Time-Dependent Orbital-Free Density Functional Theory Study with Thousands of Atoms. Journal of Physical Chemistry C, 2020, 124, 945-951.	3.1	13
23	Charge separation boosts exciton diffusion in fused ring electron acceptors. Journal of Materials Chemistry A, 2020, 8, 23304-23312.	10.3	18
24	Shedding light on moirÃ© excitons: A first-principles perspective. Science Advances, 2020, 6, .	10.3	50
25	Intramolecular Band Alignment and Spinâ€“Orbit Coupling in Two-Dimensional Halide Perovskites. Journal of Physical Chemistry Letters, 2020, 11, 6982-6989.	4.6	24
26	Excitonic Effect Drives Ultrafast Dynamics in van der Waals Heterostructures. Nano Letters, 2020, 20, 4631-4637.	9.1	46
27	AgPd nanoparticles for electrocatalytic CO₂ reduction: bimetallic composition-dependent ligand and ensemble effects. Nanoscale, 2020, 12, 14068-14075.	5.6	36
28	Band Alignment in Two-Dimensional Halide Perovskite Heterostructures: Type I or Type II?. Journal of Physical Chemistry Letters, 2020, 11, 2910-2916.	4.6	43
29	Organic Cations Protect Methylammonium Lead Iodide Perovskites against Small Exciton-Polaron Formation. Journal of Physical Chemistry Letters, 2020, 11, 2983-2991.	4.6	12
30	Impact of ball-milling and ionic liquid pretreatments on pyrolysis kinetics and behaviors of crystalline cellulose. Bioresource Technology, 2020, 305, 123044.	9.6	31
31	Reducing Anomalous Hysteresis in Perovskite Solar Cells by Suppressing the Interfacial Ferroelectric Order. ACS Applied Materials & Interfaces, 2020, 12, 12275-12284.	8.0	13
32	Zn⁺â€“O^{â€“} Dual-Spin Surface State Formation by Modification of ZnO Nanoparticles with Diboron Compounds. Langmuir, 2019, 35, 14173-14179.	3.5	5
33	Unraveling photoexcitation dynamics at â€œdots-in-a-perovskiteâ€•heterojunctions from first-principles. Journal of Materials Chemistry A, 2019, 7, 18012-18019.	10.3	12
34	In Situ Self-Assembly of Ultrastable Gold Nanoparticles on Polyvinyl Alcohol Nanofibrous Mats for Use as Highly Reusable Catalysts. ACS Omega, 2019, 4, 20094-20100.	3.5	3
35	Generalized Synthetic Strategy for Transition-Metal-Doped Brookite-Phase TiO₂ Nanorods. Journal of the American Chemical Society, 2019, 141, 16548-16552.	13.7	78
36	Modification of TiO2 Nanoparticles with Organodiboron Molecules Inducing Stable Surface Ti3+ Complex. IScience, 2019, 20, 195-204.	4.1	24

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37	PdMo bimetallene for oxygen reduction catalysis. Nature, 2019, 574, 81-85.	27.8	935
38	Radiative recombination of large polarons in halide perovskites. Journal of Physics Condensed Matter, 2019, 31, 165701.	1.8	5
39	Decreasing Exciton Binding Energy in Two-Dimensional Halide Perovskites by Lead Vacancies. Journal of Physical Chemistry Letters, 2019, 10, 3820-3827.	4.6	27
40	Self-Healing of Photocurrent Degradation in Perovskite Solar Cells: The Role of Defect-Trapped Excitons. Journal of Physical Chemistry Letters, 2019, 10, 7774-7780.	4.6	23
41	Phase Transition Control for High Performance Ruddlesdenâ€“Popper Perovskite Solar Cells. Advanced Materials, 2018, 30, e1707166.	21.0	244
42	Coupled quantum mechanics/molecular mechanics modeling of metallic materials: Theory and applications. Journal of Materials Research, 2018, 33, 796-812.	2.6	4
43	How Methylammonium Cations and Chlorine Dopants Heal Defects in Lead Iodide Perovskites. Advanced Energy Materials, 2018, 8, 1702754.	19.5	86
44	Stable Highâ€Index Faceted Pt Skin on Zigzagâ€Like PtFe Nanowires Enhances Oxygen Reduction Catalysis. Advanced Materials, 2018, 30, 1705515.	21.0	305
45	Stable Highâ€Performance Perovskite Solar Cells via Grain Boundary Passivation. Advanced Materials, 2018, 30, e1706576.	21.0	665
46	Macro-micron-nano-featured surface topography of Ti-6Al-4V alloy for biomedical applications. Rare Metals, 2018, 37, 1055-1063.	7.1	26
47	Favorable Core/Shell Interface within Co₂P/Pt Nanorods for Oxygen Reduction Electrocatalysis. Nano Letters, 2018, 18, 7870-7875.	9.1	68
48	First-order nonadiabatic couplings in extended systems by time-dependent density functional theory. Journal of Chemical Physics, 2018, 149, 244103.	3.0	8
49	Multi-inch single-crystalline perovskite membrane for high-detectivity flexible photosensors. Nature Communications, 2018, 9, 5302.	12.8	212
50	Healing detrimental defects in two-dimensional semiconductors through strain engineering. Semiconductor Science and Technology, 2018, 33, 075005.	2.0	0
51	A 1300 mm² Ultrahighâ€Performance Digital Imaging Assembly using Highâ€Quality Perovskite Single Crystals. Advanced Materials, 2018, 30, e1707314.	21.0	246
52	Large-scaleab initiocalculations of Raman scattering spectra within time-dependent density functional perturbation theory. Journal of Chemical Physics, 2018, 148, 244103.	3.0	5
53	Ultrathin PtPdâ€Based Nanorings with Abundant Step Atoms Enhance Oxygen Catalysis. Advanced Materials, 2018, 30, e1802136.	21.0	107
54	Optically inactive defects in monolayer and bilayer phosphorene: A first-principles study. Physical Review Materials, 2018, 2, .	2.4	21

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55	Multiscale Computational Design of Core/Shell Nanoparticles for Oxygen Reduction Reaction. Journal of Physical Chemistry C, 2017, 121, 1964-1973.	3.1	27
56	Probing the Bi-directional Interaction Between Microglia and Gliomas in a Tumor Microenvironment on a Microdevice. Neurochemical Research, 2017, 42, 1478-1487.	3.3	12
57	Precise tuning in platinum-nickel/nickel sulfide interface nanowires for synergistic hydrogen evolution catalysis. Nature Communications, 2017, 8, 14580.	12.8	648
58	Efficient oxygen reduction catalysis by subnanometer Pt alloy nanowires. Science Advances, 2017, 3, e1601705.	10.3	330
59	Plasmonic resonances of nanoparticles from large-scale quantum mechanical simulations. International Journal of Modern Physics B, 2017, 31, 1740003.	2.0	5
60	Effect of Point Defects on Optical Properties of Graphene Fluoride: A First-Principles Study. Journal of Physical Chemistry C, 2017, 121, 12855-12862.	3.1	30
61	Stable high efficiency two-dimensional perovskite solar cells via cesium doping. Energy and Environmental Science, 2017, 10, 2095-2102.	30.8	588
62	Charge transport in hybrid halide perovskites. Physical Review B, 2017, 96, .	3.2	22
63	Comment on â€œLinear Scaling of the Exciton Binding Energy versus the Band Gap of Two-Dimensional Materialsâ€. Physical Review Letters, 2017, 118, 209701.	7.8	8
64	Ordered PdCuâ€Based Nanoparticles as Bifunctional Oxygenâ€Reduction and Ethanolâ€Oxidation Electrocatalysts. Angewandte Chemie, 2016, 128, 9176-9181.	2.0	56
65	Ordered PdCuâ€Based Nanoparticles as Bifunctional Oxygenâ€Reduction and Ethanolâ€Oxidation Electrocatalysts. Angewandte Chemie - International Edition, 2016, 55, 9030-9035.	13.8	278
66	Quantum electrodynamics and plasmonic resonance of metallic nanostructures. Journal of Physics Condensed Matter, 2016, 28, 155302.	1.8	2
67	Biaxially strained PtPb/Pt core/shell nanoplate boosts oxygen reduction catalysis. Science, 2016, 354, 1410-1414.	12.6	1,262
68	Charge Stripe Formation in Molecular Ferroelectric Organohalide Perovskites for Efficient Charge Separation. Journal of Physical Chemistry C, 2016, 120, 23969-23975.	3.1	14
69	Generalized Surface Coordination Number as an Activity Descriptor for CO₂ Reduction on Cu Surfaces. Journal of Physical Chemistry C, 2016, 120, 28125-28130.	3.1	77
70	Surface engineering of hierarchical platinum-cobalt nanowires for efficient electrocatalysis. Nature Communications, 2016, 7, 11850.	12.8	607
71	The lowest-energy charge-transfer state and its role in charge separation in organic photovoltaics. Physical Chemistry Chemical Physics, 2016, 18, 17546-17556.	2.8	17
72	Understanding Quantum Plasmonics from Time-Dependent Orbital-Free Density Functional Theory. Journal of Physical Chemistry C, 2016, 120, 14330-14336.	3.1	29

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73	Patterning hypoxic multicellular spheroids in a 3D matrix â€“ a promising method for antiâ€tumor drug screening. Biotechnology Journal, 2016, 11, 127-134.	3.5	20
74	Subspace formulation of time-dependent density functional theory for large-scale calculations. Journal of Chemical Physics, 2015, 143, 064110.	3.0	24
75	A General Method for Multimetallic Platinum Alloy Nanowires as Highly Active and Stable Oxygen Reduction Catalysts. Advanced Materials, 2015, 27, 7204-7212.	21.0	280
76	Activation of hypoxia signaling induces phenotypic transformation of glioma cells: implications for bevacizumab antiangiogenic therapy. Oncotarget, 2015, 6, 11882-11893.	1.8	68
77	Microdevices: Flexible Fabrication of Shapeâ€Controlled Collagen Building Blocks for Selfâ€Assembly of 3D Microtissues (Small 30/2015). Small, 2015, 11, 3665-3665.	10.0	2
78	Chemical tuning of band alignments for Cu/HfO2 interfaces. Physica Status Solidi (B): Basic Research, 2015, 252, 298-304.	1.5	3
79	Do â€œHotâ€•Charge-Transfer Excitons Promote Free Carrier Generation in Organic Photovoltaics?. Journal of Physical Chemistry C, 2015, 119, 15028-15035.	3.1	27
80	Flexible Fabrication of Shapeâ€Controlled Collagen Building Blocks for Selfâ€Assembly of 3D Microtissues. Small, 2015, 11, 3666-3675.	10.0	24
81	A New Core/Shell NiAu/Au Nanoparticle Catalyst with Pt-like Activity for Hydrogen Evolution Reaction. Journal of the American Chemical Society, 2015, 137, 5859-5862.	13.7	274
82	Core/Shell Face-Centered Tetragonal FePd/Pd Nanoparticles as an Efficient Non-Pt Catalyst for the Oxygen Reduction Reaction. ACS Nano, 2015, 9, 11014-11022.	14.6	165
83	Overpotential for CO₂ electroreduction lowered on strained penta-twinned Cu nanowires. Chemical Science, 2015, 6, 6829-6835.	7.4	60
84	Strongly Interacting C₆₀/Ir(111) Interface: Transformation of C₆₀ into Graphene and Influence of Graphene Interlayer. Journal of Physical Chemistry C, 2015, 119, 27550-27555.	3.1	13
85	Effects of oxygen on prismatic faults in Î±-Ti: a combined quantum mechanics/molecular mechanics study. Scripta Materialia, 2015, 98, 32-35.	5.2	21
86	Understanding molecular structure dependence of exciton diffusion in conjugated small molecules. Applied Physics Letters, 2014, 104, 143303.	3.3	7
87	Helium bubble nucleation and growth in Î±-Fe: insights from firstâ€“principles simulations. Journal of Physics Condensed Matter, 2014, 26, 255401.	1.8	14
88	Computational Design of Core/Shell Nanoparticles for Oxygen Reduction Reactions. Journal of Physical Chemistry Letters, 2014, 5, 292-297.	4.6	71
89	Charge Separation and Exciton Dynamics at Polymer/ZnO Interface from First-Principles Simulations. Journal of Physical Chemistry Letters, 2014, 5, 2649-2656.	4.6	48
90	Size-Dependent Plasmonic Resonances from Large-Scale Quantum Simulations. Journal of Physical Chemistry Letters, 2014, 5, 1163-1169.	4.6	41

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91	Nanocatalyst Superior to Pt for Oxygen Reduction Reactions: The Case of Core/Shell Ag(Au)/CuPd Nanoparticles. Journal of the American Chemical Society, 2014, 136, 15026-15033.	13.7	172
92	Exciton diffusion in disordered small molecules for organic photovoltaics: insights from first-principles simulations. Journal of Physics Condensed Matter, 2014, 26, 185006.	1.8	8
93	Tuning Nanoparticle Structure and Surface Strain for Catalysis Optimization. Journal of the American Chemical Society, 2014, 136, 7734-7739.	13.7	349
94	Hole Transport in Diketopyrrolopyrrole (DPP) Small Molecules: A Joint Theoretical and Experimental Study. Journal of Physical Chemistry C, 2013, 117, 6730-6740.	3.1	21
95	Atomistic study of plastic deformation in Mgâ€"Al alloys. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2013, 586, 245-252.	5.6	30
96	How Cr changes the dislocation core structure of Î±-Fe: the role of magnetism. Journal of Physics Condensed Matter, 2013, 25, 085403.	1.8	1
97	Multiscale quantum/atomistic coupling using constrained density functional theory. Physical Review B, 2013, 87, .	3.2	32
98	A non-self-consistent range-separated time-dependent density functional approach for large-scale simulations. Journal of Physics Condensed Matter, 2012, 24, 205801.	1.8	20
99	First-Principles Study of Electron Mobility in Cationic and Anionic Conjugated Polyelectrolytes. Journal of Physical Chemistry C, 2012, 116, 1205-1210.	3.1	8
100	Flexible Generation of Gradient Electrospinning Nanofibers Using a Microfluidic Assisted Approach. Langmuir, 2012, 28, 10026-10032.	3.5	53
101	Dipole-Assisted Charge Separation in Organicâ€"Inorganic Hybrid Photovoltaic Heterojunctions: Insight from First-Principles Simulations. Journal of Physical Chemistry C, 2012, 116, 9845-9851.	3.1	25
102	First-principles simulations of exciton diffusion in organic semiconductors. Physical Review B, 2011, 84, .	3.2	58
103	A Fortran program for calculating electron or hole mobility in disordered semiconductors from first-principles. Computer Physics Communications, 2011, 182, 2632-2637.	7.5	6
104	Dynamic kinetic energy potential for orbital-free density functional theory. Journal of Chemical Physics, 2011, 134, 144101.	3.0	27
105	Electron structure and dynamics at poly(3-hexylthiophene)/fullerene photovoltaic heterojunctions. Applied Physics Letters, 2011, 98, 083303.	3.3	12
106	Recent Development in Quantum Mechanics/Molecular Mechanics Modeling for Materials. International Journal for Multiscale Computational Engineering, 2011, , .	1.2	1
107	Quantum mechanical study of solid solution effects on dislocation nucleation during nanoindentation. Modelling and Simulation in Materials Science and Engineering, 2010, 18, 075003.	2.0	10
108	Structure, mechanical and thermodynamic stability of vacancy clusters in Cu. Modelling and Simulation in Materials Science and Engineering, 2010, 18, 055009.	2.0	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.	2.6	28
110	Calculation of fast pipe diffusion along a dislocation stacking fault ribbon. Physical Review B, 2010, 82, .	3.2	19
111	Quantum mechanical simulations of nanoindentation of Al thin film. Computational Materials Science, 2010, 47, 769-774.	3.0	10
112	First-principles determination of charge carrier mobility in disordered semiconducting polymers. Physical Review B, 2010, 82, .	3.2	26
113	Self-consistent embedding quantum mechanics/molecular mechanics method with applications to metals. Physical Review B, 2010, 82, .	3.2	15
114	First-principles study of vacancy formation and migration in clean and Re-doped Î³â€²-Ni3Al. Acta Materialia, 2009, 57, 224-231.	7.9	27
115	Application of a hybrid quantum mechanics and empirical moleculardynamics multiscale method to carbon nanotubes. European Physical Journal B, 2008, 65, 515-523.	1.5	3
116	Transport properties of an armchair carbon nanotube with a double vacancy under stretching. Journal of Physics Condensed Matter, 2008, 20, 345225.	1.8	2
117	Electronic origin of void formation in fcc metals. Physical Review B, 2008, 77, .	3.2	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.	2.5	5
119	Quantum simulation of materials at micron scales and beyond. Physical Review B, 2008, 78, .	3.2	33
120	Electronic structure analysis of self-consistent embedding theory for quantum/molecular mechanics simulations. Physical Review B, 2008, 78, .	3.2	14
121	Quantum mechanics/molecular mechanics methodology for metals based on orbital-free density functional theory. Physical Review B, 2007, 76, .	3.2	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, , .	3.1	4