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	Biaxially strained PtPb/Pt core/shell nanoplate boosts oxygen reduction catalysis. Science, 2016, 354, 1410-1414.	6.0	1,262
2	PdMo bimetallene for oxygen reduction catalysis. Nature, 2019, 574, 81-85.	13.7	935
3	Stable Highâ€Performance Perovskite Solar Cells via Grain Boundary Passivation. Advanced Materials, 2018, 30, e1706576.	11.1	665
4	Precise tuning in platinum-nickel/nickel sulfide interface nanowires for synergistic hydrogen evolution catalysis. Nature Communications, 2017, 8, 14580.	5.8	648
5	Surface engineering of hierarchical platinum-cobalt nanowires for efficient electrocatalysis. Nature Communications, 2016, 7, 11850.	5.8	607
6	Stable high efficiency two-dimensional perovskite solar cells via cesium doping. Energy and Environmental Science, 2017, 10, 2095-2102.	15.6	588
7	Tuning Nanoparticle Structure and Surface Strain for Catalysis Optimization. Journal of the American Chemical Society, 2014, 136, 7734-7739.	6.6	349
8	Efficient oxygen reduction catalysis by subnanometer Pt alloy nanowires. Science Advances, 2017, 3, e1601705.	4.7	330
9	Stable Highâ€Index Faceted Pt Skin on Zigzagâ€Like PtFe Nanowires Enhances Oxygen Reduction Catalysis. Advanced Materials, 2018, 30, 1705515.	11.1	305
10	A General Method for Multimetallic Platinum Alloy Nanowires as Highly Active and Stable Oxygen Reduction Catalysts. Advanced Materials, 2015, 27, 7204-7212.	11.1	280
11	Ordered PdCuâ€Based Nanoparticles as Bifunctional Oxygenâ€Reduction and Ethanolâ€Oxidation Electrocatalysts. Angewandte Chemie - International Edition, 2016, 55, 9030-9035.	7.2	278
12	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.	6.6	274
13	A 1300 mm² Ultrahighâ€Performance Digital Imaging Assembly using Highâ€Quality Perovskite Single Crystals. Advanced Materials, 2018, 30, e1707314.	11.1	246
14	Phase Transition Control for High Performance Ruddlesdenâ€“Popper Perovskite Solar Cells. Advanced Materials, 2018, 30, e1707166.	11.1	244
15	Multi-inch single-crystalline perovskite membrane for high-detectivity flexible photosensors. Nature Communications, 2018, 9, 5302.	5.8	212
16	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.	6.6	172
17	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.	7.3	165
18	Ultrathin PtPdâ€Based Nanorings with Abundant Step Atoms Enhance Oxygen Catalysis. Advanced Materials, 2018, 30, e1802136.	11.1	107

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19	SARS-CoV-2 induced intestinal responses with a biomimetic human gut-on-chip. Science Bulletin, 2021, 66, 783-793.	4.3	91
20	How Methylammonium Cations and Chlorine Dopants Heal Defects in Lead Iodide Perovskites. Advanced Energy Materials, 2018, 8, 1702754.	10.2	86
21	Generalized Synthetic Strategy for Transition-Metal-Doped Brookite-Phase TiO₂ Nanorods. Journal of the American Chemical Society, 2019, 141, 16548-16552.	6.6	78
22	Generalized Surface Coordination Number as an Activity Descriptor for CO₂ Reduction on Cu Surfaces. Journal of Physical Chemistry C, 2016, 120, 28125-28130.	1.5	77
23	Computational Design of Core/Shell Nanoparticles for Oxygen Reduction Reactions. Journal of Physical Chemistry Letters, 2014, 5, 292-297.	2.1	71
24	Activation of hypoxia signaling induces phenotypic transformation of glioma cells: implications for bevacizumab antiangiogenic therapy. Oncotarget, 2015, 6, 11882-11893.	0.8	68
25	Favorable Core/Shell Interface within Co₂P/Pt Nanorods for Oxygen Reduction Electrocatalysis. Nano Letters, 2018, 18, 7870-7875.	4.5	68
26	Overpotential for CO₂ electroreduction lowered on strained penta-twinned Cu nanowires. Chemical Science, 2015, 6, 6829-6835.	3.7	60
27	First-principles simulations of exciton diffusion in organic semiconductors. Physical Review B, 2011, 84, .	1.1	58
28	Ordered PdCuâ€Based Nanoparticles as Bifunctional Oxygenâ€Reduction and Ethanolâ€Oxidation Electrocatalysts. Angewandte Chemie, 2016, 128, 9176-9181.	1.6	56
29	HiPSC-derived multi-organoids-on-chip system for safety assessment of antidepressant drugs. Lab on A Chip, 2021, 21, 571-581.	3.1	56
30	Flexible Generation of Gradient Electrospinning Nanofibers Using a Microfluidic Assisted Approach. Langmuir, 2012, 28, 10026-10032.	1.6	53
31	Shedding light on moirÃ© excitons: A first-principles perspective. Science Advances, 2020, 6, .	4.7	50
32	Microengineered Multiâ€Organoid System from hiPSCs to Recapitulate Human Liverâ€Islet Axis in Normal and Type 2 Diabetes. Advanced Science, 2022, 9, e2103495.	5.6	49
33	Charge Separation and Exciton Dynamics at Polymer/ZnO Interface from First-Principles Simulations. Journal of Physical Chemistry Letters, 2014, 5, 2649-2656.	2.1	48
34	Excitonic Effect Drives Ultrafast Dynamics in van der Waals Heterostructures. Nano Letters, 2020, 20, 4631-4637.	4.5	46
35	Band Alignment in Two-Dimensional Halide Perovskite Heterostructures: Type I or Type II?. Journal of Physical Chemistry Letters, 2020, 11, 2910-2916.	2.1	43
36	Size-Dependent Plasmonic Resonances from Large-Scale Quantum Simulations. Journal of Physical Chemistry Letters, 2014, 5, 1163-1169.	2.1	41

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37	AgPd nanoparticles for electrocatalytic CO₂ reduction: bimetallic composition-dependent ligand and ensemble effects. Nanoscale, 2020, 12, 14068-14075.	2.8	36
38	Quantum simulation of materials at micron scales and beyond. Physical Review B, 2008, 78, .	1.1	33
39	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.	3.1	33
40	Multiscale quantum/atomistic coupling using constrained density functional theory. Physical Review B, 2013, 87, .	1.1	32
41	Impact of ball-milling and ionic liquid pretreatments on pyrolysis kinetics and behaviors of crystalline cellulose. Bioresource Technology, 2020, 305, 123044.	4.8	31
42	Atomistic study of plastic deformation in Mgâ€“Al alloys. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2013, 586, 245-252.	2.6	30
43	Effect of Point Defects on Optical Properties of Graphene Fluoride: A First-Principles Study. Journal of Physical Chemistry C, 2017, 121, 12855-12862.	1.5	30
44	Understanding Quantum Plasmonics from Time-Dependent Orbital-Free Density Functional Theory. Journal of Physical Chemistry C, 2016, 120, 14330-14336.	1.5	29
45	Angstrom-Scale Spectroscopic Visualization of Interfacial Interactions in an Organic/Borophene Vertical Heterostructure. Journal of the American Chemical Society, 2021, 143, 15624-15634.	6.6	29
46	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
47	First-principles study of vacancy formation and migration in clean and Re-doped Î³â€²-Ni3Al. Acta Materialia, 2009, 57, 224-231.	3.8	27
48	Dynamic kinetic energy potential for orbital-free density functional theory. Journal of Chemical Physics, 2011, 134, 144101.	1.2	27
49	Do â€œHotâ€•Charge-Transfer Excitons Promote Free Carrier Generation in Organic Photovoltaics?. Journal of Physical Chemistry C, 2015, 119, 15028-15035.	1.5	27
50	Multiscale Computational Design of Core/Shell Nanoparticles for Oxygen Reduction Reaction. Journal of Physical Chemistry C, 2017, 121, 1964-1973.	1.5	27
51	Decreasing Exciton Binding Energy in Two-Dimensional Halide Perovskites by Lead Vacancies. Journal of Physical Chemistry Letters, 2019, 10, 3820-3827.	2.1	27
52	Quantum mechanics/molecular mechanics methodology for metals based on orbital-free density functional theory. Physical Review B, 2007, 76, .	1.1	26
53	First-principles determination of charge carrier mobility in disordered semiconducting polymers. Physical Review B, 2010, 82, .	1.1	26
54	Macro-micron-nano-featured surface topography of Ti-6Al-4V alloy for biomedical applications. Rare Metals, 2018, 37, 1055-1063.	3.6	26

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55	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.	1.5	26
56	Dipole-Assisted Charge Separation in Organicâ€“Inorganic Hybrid Photovoltaic Heterojunctions: Insight from First-Principles Simulations. Journal of Physical Chemistry C, 2012, 116, 9845-9851.	1.5	25
57	Subspace formulation of time-dependent density functional theory for large-scale calculations. Journal of Chemical Physics, 2015, 143, 064110.	1.2	24
58	Flexible Fabrication of Shapeâ€Controlled Collagen Building Blocks for Selfâ€Assembly of 3D Microtissues. Small, 2015, 11, 3666-3675.	5.2	24
59	Modification of TiO2 Nanoparticles with Organodiboron Molecules Inducing Stable Surface Ti3+ Complex. IScience, 2019, 20, 195-204.	1.9	24
60	Intramolecular Band Alignment and Spinâ€“Orbit Coupling in Two-Dimensional Halide Perovskites. Journal of Physical Chemistry Letters, 2020, 11, 6982-6989.	2.1	24
61	Self-Healing of Photocurrent Degradation in Perovskite Solar Cells: The Role of Defect-Trapped Excitons. Journal of Physical Chemistry Letters, 2019, 10, 7774-7780.	2.1	23
62	A flexible microfluidic strategy to generate grooved microfibers for guiding cell alignment. Biomaterials Science, 2021, 9, 4880-4890.	2.6	23
63	Charge transport in hybrid halide perovskites. Physical Review B, 2017, 96, .	1.1	22
64	Hole Transport in Diketopyrrolopyrrole (DPP) Small Molecules: A Joint Theoretical and Experimental Study. Journal of Physical Chemistry C, 2013, 117, 6730-6740.	1.5	21
65	Effects of oxygen on prismatic faults in Î±-Ti: a combined quantum mechanics/molecular mechanics study. Scripta Materialia, 2015, 98, 32-35.	2.6	21
66	Optically inactive defects in monolayer and bilayer phosphorene: A first-principles study. Physical Review Materials, 2018, 2, .	0.9	21
67	A non-self-consistent range-separated time-dependent density functional approach for large-scale simulations. Journal of Physics Condensed Matter, 2012, 24, 205801.	0.7	20
68	Patterning hypoxic multicellular spheroids in a 3D matrix â€“ a promising method for antiâ€tumor drug screening. Biotechnology Journal, 2016, 11, 127-134.	1.8	20
69	Calculation of fast pipe diffusion along a dislocation stacking fault ribbon. Physical Review B, 2010, 82, .	1.1	19
70	Linear-Response Time-Dependent Density Functional Theory with Stochastic Range-Separated Hybrids. Journal of Chemical Theory and Computation, 2020, 16, 1064-1072.	2.3	19
71	Data driven discovery of conjugated polyelectrolytes for optoelectronic and photocatalytic applications. Npj Computational Materials, 2021, 7, .	3.5	19
72	Charge separation boosts exciton diffusion in fused ring electron acceptors. Journal of Materials Chemistry A, 2020, 8, 23304-23312.	5.2	18

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73	Chemically identifying single adatoms with single-bond sensitivity during oxidation reactions of borophene. Nature Communications, 2022, 13, 1796.	5.8	18
74	Electronic origin of void formation in fcc metals. Physical Review B, 2008, 77, .	1.1	17
75	The lowest-energy charge-transfer state and its role in charge separation in organic photovoltaics. Physical Chemistry Chemical Physics, 2016, 18, 17546-17556.	1.3	17
76	Unraveling Structural and Optical Properties of Two-Dimensional Mo_xW_{1â€“x}S₂ Alloys. Journal of Physical Chemistry C, 2021, 125, 774-781.	1.5	17
77	CoNi nano-alloy anchored on biomass-derived N-doped carbon frameworks for enhanced oxygen reduction and evolution reactions. Electrochimica Acta, 2022, 402, 139555.	2.6	17
78	MoirÃ© excitons in defective van der Waals heterostructures. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	16
79	Unraveling energy and charge transfer in type-II van der Waals heterostructures. Npj Computational Materials, 2021, 7, .	3.5	16
80	Self-consistent embedding quantum mechanics/molecular mechanics method with applications to metals. Physical Review B, 2010, 82, .	1.1	15
81	Electronic structure analysis of self-consistent embedding theory for quantum/molecular mechanics simulations. Physical Review B, 2008, 78, .	1.1	14
82	Helium bubble nucleation and growth in Î±-Fe: insights from firstâ€“principles simulations. Journal of Physics Condensed Matter, 2014, 26, 255401.	0.7	14
83	Charge Stripe Formation in Molecular Ferroelectric Organohalide Perovskites for Efficient Charge Separation. Journal of Physical Chemistry C, 2016, 120, 23969-23975.	1.5	14
84	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.	6.6	14
85	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.	1.5	13
86	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.	1.5	13
87	Reducing Anomalous Hysteresis in Perovskite Solar Cells by Suppressing the Interfacial Ferroelectric Order. ACS Applied Materials & Interfaces, 2020, 12, 12275-12284.	4.0	13
88	Electron structure and dynamics at poly(3-hexylthiophene)/fullerene photovoltaic heterojunctions. Applied Physics Letters, 2011, 98, 083303.	1.5	12
89	Probing the Bi-directional Interaction Between Microglia and Gliomas in a Tumor Microenvironment on a Microdevice. Neurochemical Research, 2017, 42, 1478-1487.	1.6	12
90	Unraveling photoexcitation dynamics at â€œdots-in-a-perovskiteâ€•heterojunctions from first-principles. Journal of Materials Chemistry A, 2019, 7, 18012-18019.	5.2	12

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91	Organic Cations Protect Methylammonium Lead Iodide Perovskites against Small Exciton-Polaron Formation. Journal of Physical Chemistry Letters, 2020, 11, 2983-2991.	2.1	12
92	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.	2.2	12
93	Quantum mechanical study of solid solution effects on dislocation nucleation during nanoindentation. Modelling and Simulation in Materials Science and Engineering, 2010, 18, 075003.	0.8	10
94	Structure, mechanical and thermodynamic stability of vacancy clusters in Cu. Modelling and Simulation in Materials Science and Engineering, 2010, 18, 055009.	0.8	10
95	Quantum mechanical simulations of nanoindentation of Al thin film. Computational Materials Science, 2010, 47, 769-774.	1.4	10
96	First-Principles Study of Electron Mobility in Cationic and Anionic Conjugated Polyelectrolytes. Journal of Physical Chemistry C, 2012, 116, 1205-1210.	1.5	8
97	Exciton diffusion in disordered small molecules for organic photovoltaics: insights from first-principles simulations. Journal of Physics Condensed Matter, 2014, 26, 185006.	0.7	8
98	Comment on â€œLinear Scaling of the Exciton Binding Energy versus the Band Gap of Two-Dimensional Materialsâ€• Physical Review Letters, 2017, 118, 209701.	2.9	8
99	First-order nonadiabatic couplings in extended systems by time-dependent density functional theory. Journal of Chemical Physics, 2018, 149, 244103.	1.2	8
100	Understanding molecular structure dependence of exciton diffusion in conjugated small molecules. Applied Physics Letters, 2014, 104, 143303.	1.5	7
101	A Fortran program for calculating electron or hole mobility in disordered semiconductors from first-principles. Computer Physics Communications, 2011, 182, 2632-2637.	3.0	6
102	One-Dimensional Flat Bands and Anisotropic MoirÃ© Excitons in Twisted Tin Sulfide Bilayers. Chemistry of Materials, 2021, 33, 7432-7440.	3.2	6
103	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
104	Plasmonic resonances of nanoparticles from large-scale quantum mechanical simulations. International Journal of Modern Physics B, 2017, 31, 1740003.	1.0	5
105	Large-scaleab initiocalculations of Raman scattering spectra within time-dependent density functional perturbation theory. Journal of Chemical Physics, 2018, 148, 244103.	1.2	5
106	Zn⁺â€“O^{â€“} Dual-Spin Surface State Formation by Modification of ZnO Nanoparticles with Diboron Compounds. Langmuir, 2019, 35, 14173-14179.	1.6	5
107	Radiative recombination of large polarons in halide perovskites. Journal of Physics Condensed Matter, 2019, 31, 165701.	0.7	5
108	Predictions of moirÃ© excitons in twisted two-dimensional organicâ€“inorganic halide perovskites. Chemical Science, 2021, 12, 6073-6080.	3.7	5

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109	Coupled quantum mechanics/molecular mechanics modeling of metallic materials: Theory and applications. Journal of Materials Research, 2018, 33, 796-812.	1.2	4
110	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
111	Application of a hybrid quantum mechanics and empirical moleculardynamics multiscale method to carbon nanotubes. European Physical Journal B, 2008, 65, 515-523.	0.6	3
112	Chemical tuning of band alignments for Cu/HfO2 interfaces. Physica Status Solidi (B): Basic Research, 2015, 252, 298-304.	0.7	3
113	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.	1.6	3
114	Understanding Quantum Plasmonic Enhancement in Nanorod Dimers from Time-Dependent Orbital-Free Density Functional Theory. Journal of Physical Chemistry C, 2022, 126, 5046-5054.	1.5	3
115	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.	2.1	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	Microdevices: Flexible Fabrication of Shapeâ€Controlled Collagen Building Blocks for Selfâ€Assembly of 3D Microtissues (Small 30/2015). Small, 2015, 11, 3665-3665.	5.2	2
118	Quantum electrodynamics and plasmonic resonance of metallic nanostructures. Journal of Physics Condensed Matter, 2016, 28, 155302.	0.7	2
119	Frenkel defects promote polaronic exciton dissociation in methylammonium lead iodide perovskites. Physical Chemistry Chemical Physics, 2021, 23, 6583-6590.	1.3	2
120	How Cr changes the dislocation core structure of Î±-Fe: the role of magnetism. Journal of Physics Condensed Matter, 2013, 25, 085403.	0.7	1
121	Recent Development in Quantum Mechanics/Molecular Mechanics Modeling for Materials. International Journal for Multiscale Computational Engineering, 2011, , .	0.8	1
122	Healing detrimental defects in two-dimensional semiconductors through strain engineering. Semiconductor Science and Technology, 2018, 33, 075005.	1.0	0