Yan-Ning Zhang

List of Publications by Year
in descending order

102 papers	4,221 citations	101543 36 h-index	118850 62 g-index
102 all docs	102 docs citations	102 times ranked	6012 citing authors

#	Article	IF	Citations
1	Greatly Improving Electrochemical N₂ Reduction over TiO₂ Nanoparticles by Iron Doping. Angewandte Chemie - International Edition, 2019, 58, 18449-18453.	13.8	379
2	Identifying the Origin of Ti³⁺ Activity toward Enhanced Electrocatalytic N₂ Reduction over TiO₂ Nanoparticles Modulated by Mixedâ€Valent Copper. Advanced Materials, 2020, 32, e2000299.	21.0	278
3	Boron Nanosheet: An Elemental Two-Dimensional (2D) Material for Ambient Electrocatalytic N₂-to-NH₃ Fixation in Neutral Media. ACS Catalysis, 2019, 9, 4609-4615.	11.2	253
4	First-Principles Study of Lead Iodide Perovskite Tetragonal and Orthorhombic Phases for Photovoltaics. Journal of Physical Chemistry C, 2014, 118, 19565-19571.	3.1	220
5	Promoting Formation of Oxygen Vacancies in Two-Dimensional Cobalt-Doped Ceria Nanosheets for Efficient Hydrogen Evolution. Journal of the American Chemical Society, 2020, 142, 6461-6466.	13.7	168
6	Iron Pyrite Thin Films Synthesized from an Fe(acac)₃ Ink. Journal of the American Chemical Society, 2013, 135, 4412-4424.	13.7	140
7	Insights into defective TiO₂ in electrocatalytic N₂ reduction: combining theoretical and experimental studies. Nanoscale, 2019, 11, 1555-1562.	5.6	126
8	New manifold two-dimensional single-layer structures of zinc-blende compounds. Journal of Materials Chemistry A, 2014, 2, 17971-17978.	10.3	107
9	Increasing the Band Gap of Iron Pyrite by Alloying with Oxygen. Journal of the American Chemical Society, 2012, 134, 13216-13219.	13.7	96
10	Novel heterostructures by stacking layered molybdenum disulfides and nitrides for solar energy conversion. Journal of Materials Chemistry A, 2014, 2, 15389-15395.	10.3	87
11	First-principles studies of the electronic properties of native and substitutional anionic defects in bulk iron pyrite. Physical Review B, 2012, 85, .	3.2	83
12	Porous BN for hydrogen generation and storage. Journal of Materials Chemistry A, 2015, 3, 9632-9637.	10.3	83
13	Superlubricity Enabled by Pressure-Induced Friction Collapse. Journal of Physical Chemistry Letters, 2018, 9, 2554-2559.	4.6	79
14	Melting of Cu nanoclusters by molecular dynamics simulation. Physics Letters, Section A: General, Atomic and Solid State Physics, 2003, 310, 197-202.	2.1	78
15	Understanding strong magnetostriction in Fe100â^'xGax alloys. Scientific Reports, 2013, 3, 3521.	3.3	74
16	Effect of surface stoichiometry on the band gap of the pyrite FeS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>(100) surface. Physical Review B, 2012, 85, .	3.2	73
17	P-Doped graphene toward enhanced electrocatalytic N₂ reduction. Chemical Communications, 2020, 56, 1831-1834.	4.1	67
18	Greatly boosting electrochemical hydrogen evolution reaction over Ni3S2 nanosheets rationally decorated by Ni3Sn2S2 quantum dots. Applied Catalysis B: Environmental, 2020, 267, 118675.	20.2	63

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19	Electrochemical Study of Poly(2,6â€Anthraquinonyl Sulfide) as Cathode for Alkaliâ€Metalâ€Ion Batteries. Advanced Energy Materials, 2020, 10, 2002780.	19.5	60
20	Ab initio studies of the effect of nanoclusters on magnetostriction of Fe1â^'xGax alloys. Applied Physics Letters, 2010, 97, .	3.3	56
21	Interfacial Engineered Polyaniline/Sulfur-Doped TiO₂ Nanotube Arrays for Ultralong Cycle Lifetime Fiber-Shaped, Solid-State Supercapacitors. ACS Applied Materials & Interfaces, 2018, 10, 18390-18399.	8.0	56
22	Rigid band model for prediction of magnetostriction of iron-gallium alloys. Applied Physics Letters, 2010, 96, .	3.3	55
23	Anchoring and space-confinement effects to form ultrafine Ru nanoclusters for efficient hydrogen generation. Journal of Materials Chemistry A, 2018, 6, 13859-13866.	10.3	55
24	Surface Termination of Cleaved<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Bi</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi>Se</mml:mi><mml:mn	7.8	52
	by Low Energy Ion Scattering. Physical Review Letters, 2013, 110, 156101.		
25	Effect of surface composition on electronic properties of methylammonium lead iodide perovskite. Journal of Materiomics, 2015, 1, 213-220.	5.7	49
26	Hollow Bi₂MoO₆ Sphere Effectively Catalyzes the Ambient Electroreduction of N₂ to NH₃. ACS Sustainable Chemistry and Engineering, 2019, 7, 12692-12696.	6.7	49
27	Modulating Oxygen Vacancies of TiO₂ Nanospheres by Mn-Doping to Boost Electrocatalytic N₂ Reduction. ACS Sustainable Chemistry and Engineering, 2021, 9, 1512-1517.	6.7	48
28	Real-Space Imaging of Kondo Screening in a Two-Dimensional O ₂ Lattice. Science, 2011, 333, 324-328.	12.6	46
29	Influence of magnetic ordering and Jahnâ€“Teller distortion on the lithiation process of LiMn₂O₄. Physical Chemistry Chemical Physics, 2017, 19, 6481-6486.	2.8	46
30	The stability and electronic properties of novel three-dimensional graphene-MoS2 hybrid structure. Scientific Reports, 2014, 4, 7007.	3.3	45
31	Why Sliding Friction of Ne and Kr Monolayers Is So Different on the Pb(111) Surface. Physical Review Letters, 2011, 106, 236103.	7.8	44
32	Greatly Improving Electrochemical N₂ Reduction over TiO₂ Nanoparticles by Iron Doping. Angewandte Chemie, 2019, 131, 18620-18624.	2.0	44
33	High carrier mobility of few-layer PbX (X = S, Se, Te). Journal of Materials Chemistry C, 2015, 3, 6284-6290.	5.5	41
34	Interfacial engineering of Ni/V2O3 for hydrogen evolution reaction. Nano Research, 2020, 13, 2407-2412.	10.4	41
35	Direct CO Oxidation by Lattice Oxygen on Zr-Doped Ceria Surfaces. Catalysis Letters, 2011, 141, 78-82.	2.6	39
36	Modulating the phase transition between metallic and semiconducting single-layer MoS₂ and WS₂ through size effects. Physical Chemistry Chemical Physics, 2015, 17, 1099-1105.	2.8	38

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37	Pseudodielectric function and critical-point energies of iron pyrite. Physical Review B, 2012, 86, .	3.2	34
38	Understanding of large auxetic properties of iron-gallium and iron-aluminum alloys. Journal of Applied Physics, 2010, 108, .	2.5	33
39	Environmentally friendly Mn-alloyed core/shell quantum dots for high-efficiency photoelectrochemical cells. Journal of Materials Chemistry A, 2020, 8, 10736-10741.	10.3	33
40	Large magnetostriction of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Fe</mml:mtext></mml:mrow><mml:mrow><mml:mn>1</mml:mn></mml:mr its electronic origin: Density functional study. Physical Review B, 2009, 80, .	3.2	31
41	Mechanism of Large Magnetostriction of Galfenol. IEEE Transactions on Magnetics, 2011, 47, 4044-4049.	2.1	31
42	Magnetocrystalline anisotropy of Fe-Si alloys on MgO(001). Physical Review B, 2010, 81, .	3.2	28
43	Correlating Electronic Transport to Atomic Structures in Self-Assembled Quantum Wires. Nano Letters, 2012, 12, 938-942.	9.1	28
44	Electronic structure modulation of bifunctional oxygen catalysts for rechargeable Znâ€“air batteries. Journal of Materials Chemistry A, 2020, 8, 1229-1237.	10.3	26
45	Thermodynamic, dynamic and structural relaxation in supercooled liquid and glassy Ni below the critical temperature. Journal of Physics Condensed Matter, 2007, 19, 196106.	1.8	25
46	First-principles determination of the rhombohedral magnetostriction of Fe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>100</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>Al<mm xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mi>x</mml:mi></mml:msub></mml:math>and Fe<mml:math	3.2	25
47	xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml. Thermodynamic Regulation of Dendrite-Free Li Plating on Li₃Bi for Stable Lithium Metal Batteries. Nano Letters, 2021, 21, 8664-8670.	9.1	25
48	Effect of chemical order on the magnetic and electronic properties of epitaxial off-stoichiometryFexSi1â^’xthin films. Physical Review B, 2015, 91, .	3.2	24
49	Nonvolatile electric field control of magnetism in bilayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CrI</mml:mi><mml:mn>3</mml:mn></mml:msub></mml on monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>In</mml:mi><mml:mn>2</mml:mn></mml:mr Physical Review B, 2021, 104, .	3.2	24
50	Theoretical and experimental design of Pt-Co(OH)2 electrocatalyst for efficient HER performance in alkaline solution. Progress in Natural Science: Materials International, 2019, 29, 356-361.	4.4	23
51	Nanowire Quantum Dot Surface Engineering for High Temperature Single Photon Emission. ACS Nano, 2019, 13, 13492-13500.	14.6	22
52	Unusual electrochemical N₂ reduction activity in an earth-abundant iron catalyst via phosphorous modulation. Chemical Communications, 2020, 56, 731-734.	4.1	22
53	Atomistic Modeling of Sulfur Vacancy Diffusion Near Iron Pyrite Surfaces. Journal of Physical Chemistry C, 2015, 119, 24859-24864.	3.1	21
54	Three-Dimensional Nanoporous Polyethylene-Reinforced PVDF-HFP Separator Enabled by Dual-Solvent Hierarchical Gas Liberation for Ultrahigh-Rate Lithium Ion Batteries. ACS Applied Energy Materials, 2018, 1, 921-927.	5.1	21

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55	Two-dimensional square-pyramidal VO₂ with tunable electronic properties. Journal of Materials Chemistry C, 2015, 3, 3189-3197.	5.5	20
56	Pressure effect on the structural transition of liquid Au. Physics Letters, Section A: General, Atomic and Solid State Physics, 2004, 320, 452-458.	2.1	19
57	Bismuth germanate (Bi₄Ge₃O₁₂), a promising high-capacity lithium-ion battery anode. Chemical Communications, 2018, 54, 11483-11486.	4.1	19
58	Effects of van der Waals Dispersion Interactions in Density Functional Studies of Adsorption, Catalysis, and Tribology on Metals. Journal of Physical Chemistry C, 2020, 124, 16926-16942.	3.1	19
59	Attraction induced frictionless sliding of rare gas monolayer on metallic surfaces: an efficient strategy for superlubricity. Physical Chemistry Chemical Physics, 2017, 19, 11026-11031.	2.8	18
60	A critical transition state in liquid metals. Materials Letters, 2007, 61, 2434-2438.	2.6	17
61	Induced magnetism on silicon in Fe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>Si quasi-Heusler compound. Physical Review B, 2012, 85, .	3.2	17
62	First-Principles Studies on the Structural Stability of Spinel ZnCo2O4 as an Electrode Material for Lithium-ion Batteries. Scientific Reports, 2016, 6, 36717.	3.3	17
63	Relating nucleation to dynamical and structural heterogeneity in supercooled liquid metal. Physics Letters, Section A: General, Atomic and Solid State Physics, 2006, 350, 69-74.	2.1	16
64	First-principles studies on the electronic and optical properties of Fe-doped potassium dihydrogen phosphate crystal. Computational Materials Science, 2018, 143, 398-402.	3.0	16
65	Large magnetostriction in Fe-based alloys predicted by density functional theory. Physical Review B, 2010, 82, .	3.2	15
66	Structural simulation of super-cooled liquid Auâ€“Cu, Auâ€“Ag alloys. Physics Letters, Section A: General, Atomic and Solid State Physics, 2003, 317, 489-494.	2.1	13
67	Enhanced Absorption and Diffusion Properties of Lithium on B,N,VC-decorated Graphene. Scientific Reports, 2016, 6, 37911.	3.3	13
68	How Vertical Compression Triggers Lateral Interlayer Slide for Metallic Molybdenum Disulfide?. Tribology Letters, 2018, 66, 1.	2.6	13
69	Vitrification and crystallization of metallic liquid under pressures. Journal of Physics Condensed Matter, 2006, 18, 7559-7568.	1.8	12
70	Medium-range structural order in liquid Ni20Al80 alloy: Experimental and molecular dynamics studies. Physics Letters, Section A: General, Atomic and Solid State Physics, 2006, 350, 405-409.	2.1	11
71	Using structural disorder to enhance the magnetism and spin-polarization in FexSi1 â^'xthin films for spintronics. Materials Research Express, 2014, 1, 026102.	1.6	11
72	The electrochemical properties of Co₃O₄ as a lithium-ion battery electrode: a first-principles study. Physical Chemistry Chemical Physics, 2018, 20, 25016-25022.	2.8	11

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73	Determination of corrugation and friction of Cu(111) toward adsorption and motion of Ne and Xe. Physical Review B, 2014, 89, .	3.2	10
74	Communication: Surface stability and topological surface states of cleaved Bi2Se3: First-principles studies. Journal of Chemical Physics, 2015, 143, 151101.	3.0	10
75	Theoretical Progress on the Relationship between the Structures and Properties of Perovskite Solar Cells. Advanced Theory and Simulations, 2020, 3, 2000022.	2.8	10
76	Structure and dynamics of gold nanocluster under cooling conditions. Modelling and Simulation in Materials Science and Engineering, 2004, 12, 373-379.	2.0	9
77	Medium-range order of liquid metal in the quenched state. Physica B: Condensed Matter, 2005, 355, 140-146.	2.7	9
78	Relaxation, crystallization, and glass transition in supercooled liquid Ni. Physics Letters, Section A: General, Atomic and Solid State Physics, 2008, 372, 690-694.	2.1	8
79	Magnetostriction, elasticity, and D03 phase stability in Feâ€“Ga and Feâ€“Gaâ€“Ge alloys. Journal of Applied Physics, 2011, 109, 07A904.	2.5	8
80	Monometallic nanoporous nickel with high catalytic performance towards hydrazine electro-conversion and its DFT calculations. Electrochimica Acta, 2019, 317, 449-458.	5.2	8
81	Magnetism modulation of Co₃S₄ towards the efficient hydrogen evolution reaction. Molecular Systems Design and Engineering, 2020, 5, 565-572.	3.4	8
82	The structure and transport property of liquid Al with different EAM model. Physica B: Condensed Matter, 2004, 351, 208-212.	2.7	6
83	First-principle studies on the influence of anisotropic pressure on the physical properties of aluminum nitride. Materials Research Express, 2017, 4, 016303.	1.6	6
84	Efficient Alkaline Water Oxidation with a Regenerable Nickel Pseudo-Complex. ACS Applied Materials & Interfaces, 2021, 13, 48661-48668.	8.0	6
85	Defects and impurities induced structural and electronic changes in pyrite CoS₂: first principles studies. Physical Chemistry Chemical Physics, 2018, 20, 11649-11655.	2.8	5
86	Reversible dual anionic-redox chemistry in NaCrSSe with fast charging capability. Journal of Power Sources, 2021, 502, 230022.	7.8	5
87	Mechanical behavior and auxetic properties of galfenol. Proceedings of SPIE, 2009, , .	0.8	4
88	Structural and Chemical Properties of Gold Rare Earth Disilicide Coreaˆ”Shell Nanowires. ACS Nano, 2011, 5, 477-485.	14.6	4
89	Mechanics of surface crosslinked poly(dimethyl siloxane) microstructure used for microcontact transfer printing. Journal of Applied Polymer Science, 2017, 134, 45166.	2.6	4
90	Magnetic and electronic properties of Î±-U2N3 and its role in preventing uranium from oxidation: First-principles studies. Journal of Nuclear Materials, 2018, 512, 72-78.	2.7	4

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91	Effect of structural disordering on magnetic and magneto-optical properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">F</mml:mi><mml:msub><mml:mi mathvariant="normal">e</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mi>Si</mml:mi></mml:mrow></mml:math>. Physical Review Materials, 2019, 3, .	2.4	4
92	Intrinsically Conductive Organoâ€“Silver Linear Chain Polymers [â^'Sâ€“Agâ€“Sâ€“Biphenylâ^'] _n Assembled on Roughened Elemental Silver. Journal of Physical Chemistry C, 2014, 118, 29287-29293.	3.1	3
93	Strain induced structural phase transition in TM6X6 (TM = Mo, W; X = S, Se, Te) nanowires. Journal of Solid State Chemistry, 2021, 300, 122194.	2.9	3
94	The activity evidence of Ti defect towards electrocatalytic N₂ reduction. Journal of Physics Condensed Matter, 2022, 34, 044004.	1.8	3
95	Construction of stable Mo_xS_y/CeO₂ heterostructures for the electrocatalytic hydrogen evolution reaction. Physical Chemistry Chemical Physics, 2022, 24, 4891-4898.	2.8	3
96	Influence of graphene coating on the adsorption and tribology of Xe on Au(1â€‰1â€‰1) substrate. Journal of Physics Condensed Matter, 2014, 26, 445003.	1.8	2
97	Two-dimensional hexagonal V₂O nanosheet and nanoribbons. Applied Physics Express, 2015, 8, 035201.	2.4	2
98	First-principles view of the interaction between Li and Bi₄Ge₃O₁₂ anodes. Physical Chemistry Chemical Physics, 2020, 22, 26967-26971.	2.8	2
99	The molecular dynamics simulation of structure and transport properties of sheared super-cooled liquid metal. Physics Letters, Section A: General, Atomic and Solid State Physics, 2003, 319, 518-522.	2.1	1
100	Viscous behavior of (Sn61.9Pb38.1)100â^'xREx (, 0.1, 0.3, 1 wt%) solder alloys. Physics Letters, Section A: General, Atomic and Solid State Physics, 2008, 372, 3868-3873.	2.1	1
101	Low-dimensional ScO₂with tunable electronic and magnetic properties: first-principles studies. Journal of Physics Condensed Matter, 2016, 28, 015004.	1.8	1
102	Role of Rotation Angle and Grain Boundary in Tuning the Li Intercalation Concentration to Induce Phase Transition in Bilayer MoS₂. Journal of Physical Chemistry C, 2022, 126, 8539-8544.	3.1	1