Yan-Ning Zhang

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

99 papers	3,094 citations	31 h-index	52 g-index
102 ext. papers	3,714 ext. citations	6.3 avg, IF	5.51 L-index

#	Paper	IF	Citations
99	Greatly Improving Electrochemical N Reduction over TiO Nanoparticles by Iron Doping. *Angewandte Chemie - International Edition*, **2019**, 58, 18449-18453	16.4	250
98	First-Principles Study of Lead Iodide Perovskite Tetragonal and Orthorhombic Phases for Photovoltaics. *Journal of Physical Chemistry C*, **2014**, 118, 19565-19571	3.8	196
97	Boron Nanosheet: An Elemental Two-Dimensional (2D) Material for Ambient Electrocatalytic N2-to-NH3 Fixation in Neutral Media. *ACS Catalysis*, **2019**, 9, 4609-4615	13.1	180
96	Identifying the Origin of Ti Activity toward Enhanced Electrocatalytic N Reduction over TiO Nanoparticles Modulated by Mixed-Valent Copper. *Advanced Materials*, **2020**, 32, e2000299	24	171
95	Iron pyrite thin films synthesized from an Fe(acac)3 ink. *Journal of the American Chemical Society*, **2013**, 135, 4412-24	16.4	119
94	Insights into defective TiO in electrocatalytic N reduction: combining theoretical and experimental studies. *Nanoscale*, **2019**, 11, 1555-1562	7.7	95
93	New manifold two-dimensional single-layer structures of zinc-blende compounds. *Journal of Materials Chemistry A*, **2014**, 2, 17971-17978	13	92
92	Increasing the band gap of iron pyrite by alloying with oxygen. *Journal of the American Chemical Society*, **2012**, 134, 13216-9	16.4	83
91	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	16.4	82
90	Novel heterostructures by stacking layered molybdenum disulfides and nitrides for solar energy conversion. *Journal of Materials Chemistry A*, **2014**, 2, 15389-15395	13	71
89	First-principles studies of the electronic properties of native and substitutional anionic defects in bulk iron pyrite. *Physical Review B*, **2012**, 85,	3.3	70
88	Melting of Cu nanoclusters by molecular dynamics simulation. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2003**, 310, 197-202	2.3	70
87	Porous BN for hydrogen generation and storage. *Journal of Materials Chemistry A*, **2015**, 3, 9632-9637	13	65
86	Effect of surface stoichiometry on the band gap of the pyrite FeS2(100) surface. *Physical Review B*, **2012**, 85,	3.3	62
85	Understanding strong magnetostriction in Fe(100-x)Ga(x) alloys. *Scientific Reports*, **2013**, 3, 3521	4.9	57
84	Superlubricity Enabled by Pressure-Induced Friction Collapse. *Journal of Physical Chemistry Letters*, **2018**, 9, 2554-2559	6.4	48
83	P-Doped graphene toward enhanced electrocatalytic N reduction. *Chemical Communications*, **2020**, 56, 1831-1834	5.8	48

82	Rigid band model for prediction of magnetostriction of iron-gallium alloys. *Applied Physics Letters*, **2010**, 96, 062508	3.4	47
81	Surface termination of cleaved Bi2Se3 investigated by low energy ion scattering. *Physical Review Letters*, **2013**, 110, 156101	7.4	46
80	Ab initio studies of the effect of nanoclusters on magnetostriction of Fe1−xGax alloys. *Applied Physics Letters*, **2010**, 97, 262505	3.4	46
79	Effect of surface composition on electronic properties of methylammonium lead iodide perovskite. *Journal of Materiomics*, **2015**, 1, 213-220	6.7	42
78	Anchoring and space-confinement effects to form ultrafine Ru nanoclusters for efficient hydrogen generation. *Journal of Materials Chemistry A*, **2018**, 6, 13859-13866	13	42
77	Real-space imaging of Kondo screening in a two-dimensional O□lattice. *Science*, **2011**, 333, 324-8	33.3	42
76	Why sliding friction of Ne and Kr monolayers is so different on the Pb(111) surface. *Physical Review Letters*, **2011**, 106, 236103	7.4	39
75	Interfacial Engineered Polyaniline/Sulfur-Doped TiO Nanotube Arrays for Ultralong Cycle Lifetime Fiber-Shaped, Solid-State Supercapacitors. *ACS Applied Materials & Interfaces*, **2018**, 10, 18390-18399	9.5	38
74	Greatly boosting electrochemical hydrogen evolution reaction over Ni3S2 nanosheets rationally decorated by Ni3Sn2S2 quantum dots. *Applied Catalysis B: Environmental*, **2020**, 267, 118675	21.8	38
73	The stability and electronic properties of novel three-dimensional graphene-MoS2 hybrid structure. *Scientific Reports*, **2014**, 4, 7007	4.9	37
72	Modulating the phase transition between metallic and semiconducting single-layer MoS2 and WS2 through size effects. *Physical Chemistry Chemical Physics*, **2015**, 17, 1099-105	3.6	35
71	Influence of magnetic ordering and Jahn-Teller distortion on the lithiation process of LiMnO. *Physical Chemistry Chemical Physics*, **2017**, 19, 6481-6486	3.6	32
70	Hollow Bi2MoO6 Sphere Effectively Catalyzes the Ambient Electroreduction of N2 to NH3. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 12692-12696	8.3	31
69	Greatly Improving Electrochemical N2 Reduction over TiO2 Nanoparticles by Iron Doping. *Angewandte Chemie*, **2019**, 131, 18620-18624	3.6	31
68	Direct CO Oxidation by Lattice Oxygen on Zr-Doped Ceria Surfaces. *Catalysis Letters*, **2011**, 141, 78-82	2.8	31
67	Pseudodielectric function and critical-point energies of iron pyrite. *Physical Review B*, **2012**, 86,	3.3	31
66	High carrier mobility of few-layer PbX (X = S, Se, Te). *Journal of Materials Chemistry C*, **2015**, 3, 6284-6290	7.1	29
65	Electrochemical Study of Poly(2,6-Anthraquinonyl Sulfide) as Cathode for Alkali-Metal-Ion Batteries. *Advanced Energy Materials*, **2020**, 10, 2002780	21.8	28

64	Understanding of large auxetic properties of iron-gallium and iron-aluminum alloys. *Journal of Applied Physics*, **2010**, 108, 023513	2.5	27
63	Large magnetostriction of Fe1−xGex and its electronic origin: Density functional study. *Physical Review B*, **2009**, 80,	3.3	27
62	Correlating electronic transport to atomic structures in self-assembled quantum wires. *Nano Letters*, **2012**, 12, 938-42	11.5	26
61	Interfacial engineering of Ni/V2O3 for hydrogen evolution reaction. *Nano Research*, **2020**, 13, 2407-2412	10	24
60	Effect of chemical order on the magnetic and electronic properties of epitaxial off-stoichiometry FexSi1−x thin films. *Physical Review B*, **2015**, 91,	3.3	22
59	Magnetocrystalline anisotropy of Fe-Si alloys on MgO(001). *Physical Review B*, **2010**, 81,	3.3	22
58	. *IEEE Transactions on Magnetics*, **2011**, 47, 4044-4049	2	21
57	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	21
56	Environmentally friendly Mn-alloyed core/shell quantum dots for high-efficiency photoelectrochemical cells. *Journal of Materials Chemistry A*, **2020**, 8, 10736-10741	13	20
55	First-principles determination of the rhombohedral magnetostriction of Fe100−xAlx and Fe100−xGax alloys. *Physical Review B*, **2012**, 86,	3.3	20
54	Unusual electrochemical N reduction activity in an earth-abundant iron catalyst via phosphorous modulation. *Chemical Communications*, **2020**, 56, 731-734	5.8	19
53	Atomistic Modeling of Sulfur Vacancy Diffusion Near Iron Pyrite Surfaces. *Journal of Physical Chemistry C*, **2015**, 119, 24859-24864	3.8	18
52	Pressure effect on the structural transition of liquid Au. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2004**, 320, 452-458	2.3	18
51	Modulating Oxygen Vacancies of TiO2 Nanospheres by Mn-Doping to Boost Electrocatalytic N2 Reduction. *ACS Sustainable Chemistry and Engineering*, **2021**, 9, 1512-1517	8.3	18
50	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	6.1	17
49	A critical transition state in liquid metals. *Materials Letters*, **2007**, 61, 2434-2438	3.3	17
48	Two-dimensional square-pyramidal VO2 with tunable electronic properties. *Journal of Materials Chemistry C*, **2015**, 3, 3189-3197	7.1	16
47	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	3.6	15

46	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	2.3	15
45	Large magnetostriction in Fe-based alloys predicted by density functional theory. *Physical Review B*, **2010**, 82,	3.3	14
44	Attraction induced frictionless sliding of rare gas monolayer on metallic surfaces: an efficient strategy for superlubricity. *Physical Chemistry Chemical Physics*, **2017**, 19, 11026-11031	3.6	13
43	Nanowire Quantum Dot Surface Engineering for High Temperature Single Photon Emission. *ACS Nano*, **2019**, 13, 13492-13500	16.7	13
42	Induced magnetism on silicon in Fe3Si quasi-Heusler compound. *Physical Review B*, **2012**, 85,	3.3	13
41	Structural simulation of super-cooled liquid Au□Cu, Au□Ag alloys. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2003**, 317, 489-494	2.3	12
40	Vitrification and crystallization of metallic liquid under pressures. *Journal of Physics Condensed Matter*, **2006**, 18, 7559-68	1.8	11
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38	Electronic structure modulation of bifunctional oxygen catalysts for rechargeable Zn□ir batteries. *Journal of Materials Chemistry A*, **2020**, 8, 1229-1237	13	11
37	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	3.8	11
36	Enhanced Absorption and Diffusion Properties of Lithium on B,N,V-decorated Graphene. *Scientific Reports*, **2016**, 6, 37911	4.9	11
35	Bismuth germanate (BiGeO), a promising high-capacity lithium-ion battery anode. *Chemical Communications*, **2018**, 54, 11483-11486	5.8	11
34	First-Principles Studies on the Structural Stability of Spinel ZnCoO as an Electrode Material for Lithium-ion Batteries. *Scientific Reports*, **2016**, 6, 36717	4.9	10
33	Communication: Surface stability and topological surface states of cleaved Bi2Se3: First-principles studies. *Journal of Chemical Physics*, **2015**, 143, 151101	3.9	10
32	Using structural disorder to enhance the magnetism and spin-polarization in FexSi1 □thin films for spintronics. *Materials Research Express*, **2014**, 1, 026102	1.7	10
31	Determination of corrugation and friction of Cu(111) toward adsorption and motion of Ne and Xe. *Physical Review B*, **2014**, 89,	3.3	10
30	Structure and dynamics of gold nanocluster under cooling conditions. *Modelling and Simulation in Materials Science and Engineering*, **2004**, 12, 373-379	2	9
29	Medium-range order of liquid metal in the quenched state. *Physica B: Condensed Matter*, **2005**, 355, 140-146	1.8	9

28	How Vertical Compression Triggers Lateral Interlayer Slide for Metallic Molybdenum Disulfide?. *Tribology Letters*, **2018**, 66, 1	2.8	8
27	Relaxation, crystallization, and glass transition in supercooled liquid Ni. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2008**, 372, 690-694	2.3	8
26	First-principles studies on the electronic and optical properties of Fe-doped potassium dihydrogen phosphate crystal. *Computational Materials Science*, **2018**, 143, 398-402	3.2	8
25	The electrochemical properties of CoO as a lithium-ion battery electrode: a first-principles study. *Physical Chemistry Chemical Physics*, **2018**, 20, 25016-25022	3.6	8
24	Monometallic nanoporous nickel with high catalytic performance towards hydrazine electro-conversion and its DFT calculations. *Electrochimica Acta*, **2019**, 317, 449-458	6.7	7
23	Magnetostriction, elasticity, and D03 phase stability in Fe□Ga and Fe□Ga□ alloys. *Journal of Applied Physics*, **2011**, 109, 07A904	2.5	7
22	The structure and transport property of liquid Al with different EAM model. *Physica B: Condensed Matter*, **2004**, 351, 208-212	2.8	5
21	First-principle studies on the influence of anisotropic pressure on the physical properties of aluminum nitride. *Materials Research Express*, **2017**, 4, 016303	1.7	4
20	Theoretical Progress on the Relationship between the Structures and Properties of Perovskite Solar Cells. *Advanced Theory and Simulations*, **2020**, 3, 2000022	3.5	4
19	Magnetism modulation of Co3S4 towards the efficient hydrogen evolution reaction. *Molecular Systems Design and Engineering*, **2020**, 5, 565-572	4.6	4
18	Nonvolatile electric field control of magnetism in bilayer CrI3 on monolayer In2Se3. *Physical Review B*, **2021**, 104,	3.3	4
17	Mechanics of surface crosslinked poly(dimethyl siloxane) microstructure used for microcontact transfer printing. *Journal of Applied Polymer Science*, **2017**, 134, 45166	2.9	3
16	Defects and impurities induced structural and electronic changes in pyrite CoS: first principles studies. *Physical Chemistry Chemical Physics*, **2018**, 20, 11649-11655	3.6	3
15	Intrinsically Conductive Organo□Silver Linear Chain Polymers [□Ag□Biphenyl□]n Assembled on Roughened Elemental Silver. *Journal of Physical Chemistry C*, **2014**, 118, 29287-29293	3.8	3
14	Structural and chemical properties of gold rare earth disilicide core-shell nanowires. *ACS Nano*, **2011**, 5, 477-85	16.7	3
13	Effect of structural disordering on magnetic and magneto-optical properties of Fe3Si. *Physical Review Materials*, **2019**, 3,	3.2	3
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11	Influence of graphene coating on the adsorption and tribology of Xe on Au(1 1 1) substrate. *Journal of Physics Condensed Matter*, **2014**, 26, 445003	1.8	2

10	Mechanical behavior and auxetic properties of galfenol **2009**,		2
9	Magnetic and electronic properties of U2N3 and its role in preventing uranium from oxidation: First-principles studies. *Journal of Nuclear Materials*, **2018**, 512, 72-78	3.3	2
8	Reversible dual anionic-redox chemistry in NaCrSSe with fast charging capability. *Journal of Power Sources*, **2021**, 502, 230022	8.9	2
7	Viscous behavior of (Sn61.9Pb38.1)100REx (x=0, 0.1, 0.3, 1 wt%) solder alloys. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2008**, 372, 3868-3873	2.3	1
6	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	2.3	1
5	Efficient Alkaline Water Oxidation with a Regenerable Nickel Pseudo-Complex. *ACS Applied Materials & Interfaces*, **2021**, 13, 48661-48668	9.5	1
4	Low-dimensional ScO2 with tunable electronic and magnetic properties: first-principles studies. *Journal of Physics Condensed Matter*, **2016**, 28, 015004	1.8	1
3	Strain induced structural phase transition in TM6X6 (TM = Mo, W; X = S, Se, Te) nanowires. *Journal of Solid State Chemistry*, **2021**, 300, 122194	3.3	1
2	First-principles view of the interaction between Li and BiGeO anodes. *Physical Chemistry Chemical Physics*, **2020**, 22, 26967-26971	3.6	0
1	Two-dimensional hexagonal V2O nanosheet and nanoribbons. *Applied Physics Express*, **2015**, 8, 035201	2.4	