Xiao-Li Fan

List of Publications by Year
in descending order

75 papers	2,483 citations	218677 26 h-index	206112 48 g-index
76 all docs	76 docs citations	76 times ranked	3981 citing authors

#	Article	IF	Citations
1	MXene Nanofibers as Highly Active Catalysts for Hydrogen Evolution Reaction. ACS Sustainable Chemistry and Engineering, 2018, 6, 8976-8982.	6.7	174
2	Uncovering the Veil of the Degradation in Perovskite CH₃NH₃PbI₃ upon Humidity Exposure: A First-Principles Study. Journal of Physical Chemistry Letters, 2015, 6, 3289-3295.	4.6	171
3	Laminated Hybrid Junction of Sulfurâ€Doped TiO₂ and a Carbon Substrate Derived from Ti₃C₂ MXenes: Toward Highly Visible Lightâ€Driven Photocatalytic Hydrogen Evolution. Advanced Science, 2018, 5, 1700870.	11.2	163
4	Site-specific catalytic activity in exfoliated MoS₂single-layer polytypes for hydrogen evolution: basal plane and edges. Journal of Materials Chemistry A, 2014, 2, 20545-20551.	10.3	150
5	Ferroelectricâ€Enhanced Polysulfide Trapping for Lithiumâ€“Sulfur Battery Improvement. Advanced Materials, 2017, 29, 1604724.	21.0	149
6	Ferromagnetism in Transitional Metal-Doped MoS2 Monolayer. Nanoscale Research Letters, 2016, 11, 154.	5.7	103
7	Single Atoms on a Nitrogen-Doped Boron Phosphide Monolayer: A New Promising Bifunctional Electrocatalyst for ORR and OER. ACS Applied Materials & Interfaces, 2020, 12, 52549-52559.	8.0	95
8	Nanopolygons of Monolayer MS₂: Best Morphology and Size for HER Catalysis. Nano Letters, 2017, 17, 368-376.	9.1	91
9	Point defect structure of La-doped SrTiO3 ceramics with colossal permittivity. Acta Materialia, 2019, 164, 76-89.	7.9	78
10	Catalytic Activity of MS₂ Monolayer for Electrochemical Hydrogen Evolution. Journal of Physical Chemistry C, 2016, 120, 1623-1632.	3.1	75
11	Hybrid Polymer Membrane Functionalized PBO Fibers/Cyanate Esters Wave-Transparent Laminated Composites. Advanced Fiber Materials, 2022, 4, 520-531.	16.1	67
12	Composition Directed Generation of Reactive Oxygen Species in Irradiated Mixed Metal Sulfides Correlated with Their Photocatalytic Activities. ACS Applied Materials & Interfaces, 2015, 7, 16440-16449.	8.0	65
13	3d transitional-metal single atom catalysis toward hydrogen evolution reaction on MXenes supports. International Journal of Hydrogen Energy, 2020, 45, 14396-14406.	7.1	59
14	Sc2CO2 and Mn-doped Sc2CO2 as gas sensor materials to NO and CO: A first-principles study. Physica E: Low-Dimensional Systems and Nanostructures, 2019, 111, 84-90.	2.7	54
15	A first-principles study of Sc-decorated graphene with pyridinic-N defects for hydrogen storage. International Journal of Hydrogen Energy, 2017, 42, 3106-3113.	7.1	47
16	First principles study of structural and electronic properties of cubic phase of ZrO2 and HfO2. Physica B: Condensed Matter, 2014, 434, 7-13.	2.7	43
17	Ultrathin Polymer Film Formation by Collision-Induced Cross-Linking of Adsorbed Organic Molecules with Hyperthermal Protons. Journal of the American Chemical Society, 2004, 126, 12336-12342.	13.7	38
18	Band gap engineering of FeS₂ under biaxial strain: a first principles study. Physical Chemistry Chemical Physics, 2014, 16, 24466-24472.	2.8	38

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19	Electronic and Magnetic Properties of Defected Monolayer WSe2 with Vacancies. Nanoscale Research Letters, 2019, 14, 192.	5.7	37
20	Numerical simulation of lubrication performance on chevron textured surface under hydrodynamic lubrication. Tribology International, 2021, 154, 106704.	5.9	36
21	Strain engineering the magnetic states of vacancy-doped monolayer MoSe 2. Journal of Alloys and Compounds, 2015, 635, 307-313.	5.5	35
22	Enhanced gas-sensing performance of graphene by doping transition metal atoms: A first-principles study. Physics Letters, Section A: General, Atomic and Solid State Physics, 2018, 382, 2965-2973.	2.1	34
23	Improved catalytic performance of monolayer nano-triangles WS2 and MoS2 on HER by 3d metals doping. Computational Materials Science, 2019, 159, 333-340.	3.0	31
24	Effect of strain on the magnetic states of transition-metal atoms doped monolayer WS2. Computational Materials Science, 2016, 117, 354-360.	3.0	30
25	Role of intrinsic dipole on photocatalytic water splitting for Janus MoSSe/nitrides heterostructure: A first-principles study. Progress in Natural Science: Materials International, 2019, 29, 335-340.	4.4	28
26	Cu Anchored Ti₂NO₂ as High Performance Electrocatalyst for Oxygen Evolution Reaction: A Density Functional Theory Study. ChemCatChem, 2020, 12, 4059-4066.	3.7	27
27	High Curie temperature and carrier mobility of novel Fe, Co and Ni carbide MXenes. Nanoscale, 2020, 12, 11627-11637.	5.6	26
28	Increasing the band gap of FeS2 by alloying with Zn and applying biaxial strain: A first-principles study. Journal of Alloys and Compounds, 2015, 629, 43-48.	5.5	25
29	Calcium decorated two dimensional carbon allotropes for hydrogen storage: A first-principles study. Computational Materials Science, 2016, 124, 106-113.	3.0	25
30	Significantly improved interfacial properties and wave-transparent performance of PBO fibers/cyanate esters laminated composites via introducing a polydopamine/ZIF-8 hybrid membrane. Composites Science and Technology, 2022, 223, 109426.	7.8	24
31	First-principles study on armchair AlN nanoribbons with different edge terminations. Superlattices and Microstructures, 2014, 67, 40-46.	3.1	23
32	Tuning the electronic properties of half- and full-hydrogenated germanene by chlorination and hydroxylation: A first-principles study. Computational Materials Science, 2014, 92, 244-252.	3.0	23
33	Room-temperature preparation of trisilver-copper-sulfide/polymer based heterojunction thin film for solar cell application. Journal of Power Sources, 2015, 280, 313-319.	7.8	23
34	Asymmetric MXene/monolayer transition metal dichalcogenide heterostructures for functional applications. Npj Computational Materials, 2019, 5, .	8.7	23
35	First-principles investigations of transition-metal doped bilayer WS₂. Physical Chemistry Chemical Physics, 2016, 18, 10152-10157.	2.8	21
36	Electronic and magnetic properties of group-V TMDs monolayers with defects: A first-principles study. Computational Materials Science, 2020, 176, 109540.	3.0	20

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37	Two-dimensional intrinsic ferromagnetic half-metals: monolayers Mn3X4 (Xâ€‰=â€‰Te, Se, S). Journal of Materials Science, 2020, 55, 7680-7690.	3.7	20
38	First-Principles Study on the Stability and STM Image of Borophene. Nanoscale Research Letters, 2017, 12, 514.	5.7	19
39	Improving the comprehensive properties of PBO fibres/cyanate ester composites using a hyperbranched fluorine and epoxy containing PBO precursor. Composites Part A: Applied Science and Manufacturing, 2021, 150, 106596.	7.6	19
40	Ferromagnetic half-metal with high Curie temperature: Janus Mn2PAs monolayer. Journal of Materials Science, 2021, 56, 13215-13226.	3.7	18
41	Edges of graphene and carbon nanotubes with high catalytic performance for the oxygen reduction reaction. Physical Chemistry Chemical Physics, 2017, 19, 21003-21011.	2.8	15
42	Single transition metal atom anchored on VSe2 as electrocatalyst for nitrogen reduction reaction. Applied Surface Science, 2022, 580, 152272.	6.1	15
43	From Nondissociative to Dissociative Adsorption of Benzene-thiol on Au(111): A Density Functional Theory Study. Journal of Physical Chemistry C, 2012, 116, 1002-1011.	3.1	14
44	Exploring the catalytic activity of MXenes Mn+1CnO2 for hydrogen evolution. Journal of Materials Science, 2019, 54, 11378-11389.	3.7	14
45	Ordered double-M elements MXenes TiMC: Large in-plane stiffness and ferromagnetism. Journal of Magnetism and Magnetic Materials, 2019, 486, 165280.	2.3	14
46	Two-dimensional stable Fe-based ferromagnetic semiconductors: FeI₃ and FeI_{1.5}Cl_{1.5} monolayers. Physical Chemistry Chemical Physics, 2020, 22, 24506-24515.	2.8	13
47	Cleaving Câ€“H bonds with hyperthermal H₂: facile chemistry to cross-link organic molecules under low chemical- and energy-loads. Green Chemistry, 2014, 16, 1316-1325.	9.0	12
48	Robust Superlubricity and MoirÃ© Latticeâ€™s Size Dependence on Friction between Graphdiyne Layers. ACS Applied Materials & Interfaces, 2021, 13, 40901-40908.	8.0	12
49	Computing pKa Values with a Mixing Hamiltonian Quantum Mechanical/Molecular Mechanical Approach. Journal of Chemical Theory and Computation, 2013, 9, 4257-4265.	5.3	11
50	First-principles investigation on the interface of transition metal dichalcogenide MX2 (M = Mo, W; X =) Tj ETQq0 0 0 rgBT /Overlock 10 T	3.0	10
51	Density functional theory study of the adsorption of methanthiol on Au(111): Role of gold adatoms. Physica E: Low-Dimensional Systems and Nanostructures, 2014, 59, 248-253.	2.7	9
52	Room-temperature ferromagnetism in alkaline-earth-metal doped AlP: First-principle calculations. Computational Materials Science, 2018, 142, 338-345.	3.0	9
53	Calcia-doped ceria hybrid coating functionalized PBO fibers with excellent UV resistance and improved interfacial compatibility with cyanate ester resins. Applied Surface Science, 2021, 569, 151124.	6.1	9
54	Tunable magnetic order in two-dimensional layered GdGe₂. Journal of Materials Chemistry C, 2022, 10, 1259-1269.	5.5	9

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55	Bipolar ferromagnetic semiconductor with large magnetic moment: EuGe2 monolayer. Computational Materials Science, 2022, 213, 111611.	3.0	9
56	Structural and electronic properties of conducting Cu nanowire encapsulated in semiconducting zigzag carbon nanotubes: A firstâ€principles study. Physica Status Solidi (B): Basic Research, 2012, 249, 1033-1038.	1.5	8
57	Pmma-XO (X = C, Si, Ge) monolayer as promising anchoring materials for lithiumâ€“sulfur battery: a first-principles study. Nanotechnology, 2019, 30, 085405.	2.6	8
58	Revealing the Potential Crystal Structures of Earth-Abundant Nontoxic Photovoltaic CuBiI₄. Crystal Growth and Design, 2021, 21, 2850-2855.	3.0	8
59	Magnetic semiconducting and strain-induced semiconductingâ€“metallic transition in Cu-doped single-layer WSe2. Journal of Materials Science, 2019, 54, 529-539.	3.7	7
60	Lattice distortion-enhanced superlubricity of (Mo, X)S₂ (X = Al, Ti, Cr and V) with moirÃ© superlattice. Nanoscale, 2021, 13, 16234-16243.	5.6	6
61	Dimethyl Disulfide on Cu(111): From Nondissociative to Dissociative Adsorption. Journal of Physical Chemistry C, 2013, 117, 6587-6593.	3.1	5
62	A first-principles study on the electronic and magnetic properties of armchair SiC/AlN nanoribbons. Journal of Alloys and Compounds, 2014, 586, 176-179.	5.5	5
63	First-principles study the single-layer transition metal trihalide CrXSe₃ (Xâ€‰â€‰=â€‰â€‰Sn, Ge, Si) as monolayer ferromagnetic semiconductor. Journal of Physics Condensed Matter, 2020, 32, 085801.	1.8	5
64	Effects of Intrinsic Surface Defects on Thiophenol Self-Assembly on Au(111): Surface Structures and Reaction Mechanisms. Journal of Physical Chemistry C, 2012, 116, 19909-19917.	3.1	4
65	First-Principles Study on the Electronic and Magnetic Properties of Zigzag AlN-SiC Nanoribbons. Journal of Superconductivity and Novel Magnetism, 2014, 27, 1079-1082.	1.8	4
66	DID Code: A Bridge Connecting the Materials Genome Engineering Database with Inheritable Integrated Intelligent Manufacturing. Engineering, 2020, 6, 612-620.	6.7	4
67	Density Functional Theory Studies on the Adsorption of Methanethiol Molecule on Au(111) Surface at Different Coverage. Acta Chimica Sinica, 2013, 71, 829.	1.4	4
68	Virtual voids method to generate low-density microporous carbon structures using quenched molecular dynamics simulation. Carbon, 2021, 183, 438-448.	10.3	3
69	Self-assembled monolayers of CH3S from the adsorption of CH3SSCH3 on Au(111). Physical Chemistry Chemical Physics, 2014, 16, 2533.	2.8	2
70	Response to comment on â€œpoint defect structure of La-doped SrTiO3 ceramics with colossal permittivityâ€• Scripta Materialia, 2021, 190, 118-120.	5.2	2
71	High-temperature ferromagnetism in monolayers MnGaX3 (XÂ=ÂTe, Se). Journal of Magnetism and Magnetic Materials, 2021, 534, 168041.	2.3	2
72	Stabilization and Metallic to Semiconducting Transition in 2D Boron Sheet. Engineered Science, 2018, , .	2.3	2

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73	DENSITY FUNCTIONAL THEORY STUDIES ON THE ADSORPTION OF 4-METHYLBENZENETHIOL AND 4-ETHYLBENZENETHIOL MOLECULES ONAu(111) SURFACE. Surface Review and Letters, 2014, 21, 1450087.	1.1	1
74	3-Fold-Periodic Size-Dependence in Electronic Properties of Monolayer-TMDC Nanotriangles. Journal of Physical Chemistry Letters, 2018, 9, 1346-1352.	4.6	1
75	Effects of intrinsic defects on methanthiol monolayers on Cu(111): A density functional theory study. Journal of Chemical Physics, 2013, 138, 134708.	3.0	0