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	Hybrid Polymer Membrane Functionalized PBO Fibers/Cyanate Esters Wave-Transparent Laminated Composites. Advanced Fiber Materials, 2022, 4, 520-531.	16.1	67
2	Single transition metal atom anchored on VSe2 as electrocatalyst for nitrogen reduction reaction. Applied Surface Science, 2022, 580, 152272.	6.1	15
3	Tunable magnetic order in two-dimensional layered GdGe₂. Journal of Materials Chemistry C, 2022, 10, 1259-1269.	5.5	9
4	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
5	Bipolar ferromagnetic semiconductor with large magnetic moment: EuGe2 monolayer. Computational Materials Science, 2022, 213, 111611.	3.0	9
6	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
7	Numerical simulation of lubrication performance on chevron textured surface under hydrodynamic lubrication. Tribology International, 2021, 154, 106704.	5.9	36
8	Revealing the Potential Crystal Structures of Earth-Abundant Nontoxic Photovoltaic CuBiI₄. Crystal Growth and Design, 2021, 21, 2850-2855.	3.0	8
9	Ferromagnetic half-metal with high Curie temperature: Janus Mn2PAs monolayer. Journal of Materials Science, 2021, 56, 13215-13226.	3.7	18
10	Robust Superlubricity and MoirÃ© Latticeâ€™s Size Dependence on Friction between Graphdiyne Layers. ACS Applied Materials & Interfaces, 2021, 13, 40901-40908.	8.0	12
11	High-temperature ferromagnetism in monolayers MnGaX3 (XÂ=ÂTe, Se). Journal of Magnetism and Magnetic Materials, 2021, 534, 168041.	2.3	2
12	Virtual voids method to generate low-density microporous carbon structures using quenched molecular dynamics simulation. Carbon, 2021, 183, 438-448.	10.3	3
13	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
14	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
15	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
16	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
17	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
18	Cu Anchored Ti₂NO₂ as High Performance Electrocatalyst for Oxygen Evolution Reaction: A Density Functional Theory Study. ChemCatChem, 2020, 12, 4059-4066.	3.7	27

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19	DID Code: A Bridge Connecting the Materials Genome Engineering Database with Inheritable Integrated Intelligent Manufacturing. Engineering, 2020, 6, 612-620.	6.7	4
20	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
21	Electronic and magnetic properties of group-V TMDs monolayers with defects: A first-principles study. Computational Materials Science, 2020, 176, 109540.	3.0	20
22	High Curie temperature and carrier mobility of novel Fe, Co and Ni carbide MXenes. Nanoscale, 2020, 12, 11627-11637.	5.6	26
23	Two-dimensional intrinsic ferromagnetic half-metals: monolayers Mn3X4 (Xâ€‰=â€‰Te, Se, S). Journal of Materials Science, 2020, 55, 7680-7690.	3.7	20
24	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
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	Electronic and Magnetic Properties of Defected Monolayer WSe2 with Vacancies. Nanoscale Research Letters, 2019, 14, 192.	5.7	37
27	Exploring the catalytic activity of MXenes Mn+1CnO2 for hydrogen evolution. Journal of Materials Science, 2019, 54, 11378-11389.	3.7	14
28	Ordered double-M elements MXenes TiMC: Large in-plane stiffness and ferromagnetism. Journal of Magnetism and Magnetic Materials, 2019, 486, 165280.	2.3	14
29	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
30	Asymmetric MXene/monolayer transition metal dichalcogenide heterostructures for functional applications. Npj Computational Materials, 2019, 5, .	8.7	23
31	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
32	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
33	Point defect structure of La-doped SrTiO3 ceramics with colossal permittivity. Acta Materialia, 2019, 164, 76-89.	7.9	78
34	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
35	3-Fold-Periodic Size-Dependence in Electronic Properties of Monolayer-TMDC Nanotriangles. Journal of Physical Chemistry Letters, 2018, 9, 1346-1352.	4.6	1
36	Laminated Hybrid Junction of SulfurâĐoped TiO₂ and a Carbon Substrate Derived from Ti₃C₂ MXenes: Toward Highly Visible LightâĐriven Photocatalytic Hydrogen Evolution. Advanced Science, 2018, 5, 1700870.	11.2	163

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37	Room-temperature ferromagnetism in alkaline-earth-metal doped AlP: First-principle calculations. Computational Materials Science, 2018, 142, 338-345.	3.0	9
38	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
39	MXene Nanofibers as Highly Active Catalysts for Hydrogen Evolution Reaction. ACS Sustainable Chemistry and Engineering, 2018, 6, 8976-8982.	6.7	174
40	Stabilization and Metallic to Semiconducting Transition in 2D Boron Sheet. Engineered Science, 2018, , .	2.3	2
41	Ferroelectricâ€Enhanced Polysulfide Trapping for Lithiumâ€“Sulfur Battery Improvement. Advanced Materials, 2017, 29, 1604724.	21.0	149
42	Nanopolygons of Monolayer MS₂: Best Morphology and Size for HER Catalysis. Nano Letters, 2017, 17, 368-376.	9.1	91
43	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
44	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
45	First-Principles Study on the Stability and STM Image of Borophene. Nanoscale Research Letters, 2017, 12, 514.	5.7	19
46	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
47	Calcium decorated two dimensional carbon allotropes for hydrogen storage: A first-principles study. Computational Materials Science, 2016, 124, 106-113.	3.0	25
48	Ferromagnetism in Transitional Metal-Doped MoS2 Monolayer. Nanoscale Research Letters, 2016, 11, 154.	5.7	103
49	Catalytic Activity of MS₂ Monolayer for Electrochemical Hydrogen Evolution. Journal of Physical Chemistry C, 2016, 120, 1623-1632.	3.1	75
50	First-principles investigations of transition-metal doped bilayer WS₂. Physical Chemistry Chemical Physics, 2016, 18, 10152-10157.	2.8	21
51	Effect of strain on the magnetic states of transition-metal atoms doped monolayer WS2. Computational Materials Science, 2016, 117, 354-360.	3.0	30
52	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
53	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
54	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

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55	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
56	Strain engineering the magnetic states of vacancy-doped monolayer MoSe 2. Journal of Alloys and Compounds, 2015, 635, 307-313.	5.5	35
57	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
58	First-principles study on armchair AlN nanoribbons with different edge terminations. Superlattices and Microstructures, 2014, 67, 40-46.	3.1	23
59	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
60	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
61	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
62	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
63	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
64	Self-assembled monolayers of CH3S from the adsorption of CH3SSCH3 on Au(111). Physical Chemistry Chemical Physics, 2014, 16, 2533.	2.8	2
65	Band gap engineering of FeS₂ under biaxial strain: a first principles study. Physical Chemistry Chemical Physics, 2014, 16, 24466-24472.	2.8	38
66	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
67	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
68	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
69	Dimethyl Disulfide on Cu(111): From Nondissociative to Dissociative Adsorption. Journal of Physical Chemistry C, 2013, 117, 6587-6593.	3.1	5
70	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
71	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
72	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

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73	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
74	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
75	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