Xiao-Li Fan

List of Publications by Citations

74 papers	1,597 citations	20 h-index	38 g-index
76 ext. papers	2,026 ext. citations	5.7 avg, IF	5.04 L-index

#	Paper	IF	Citations
74	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	6.4	147
73	Site-specific catalytic activity in exfoliated MoS2 single-layer polytypes for hydrogen evolution: basal plane and edges. *Journal of Materials Chemistry A*, **2014**, 2, 20545-20551	13	127
72	Ferroelectric-Enhanced Polysulfide Trapping for Lithium-Sulfur Battery Improvement. *Advanced Materials*, **2017**, 29, 1604724	24	124
71	Laminated Hybrid Junction of Sulfur-Doped TiO and a Carbon Substrate Derived from TiC MXenes: Toward Highly Visible Light-Driven Photocatalytic Hydrogen Evolution. *Advanced Science*, **2018**, 5, 1700870	13.6	108
70	MXene Nanofibers as Highly Active Catalysts for Hydrogen Evolution Reaction. *ACS Sustainable Chemistry and Engineering*, **2018**, 6, 8976-8982	8.3	103
69	Ferromagnetism in Transitional Metal-Doped MoS2 Monolayer. *Nanoscale Research Letters*, **2016**, 11, 154	5	75
68	Nanopolygons of Monolayer MS: Best Morphology and Size for HER Catalysis. *Nano Letters*, **2017**, 17, 368-376	11.5	71
67	Catalytic Activity of MS2 Monolayer for Electrochemical Hydrogen Evolution. *Journal of Physical Chemistry C*, **2016**, 120, 1623-1632	3.8	67
66	Composition Directed Generation of Reactive Oxygen Species in Irradiated Mixed Metal Sulfides Correlated with Their Photocatalytic Activities. *ACS Applied Materials & Interfaces*, **2015**, 7, 16440-9	9.5	52
65	Point defect structure of La-doped SrTiO3 ceramics with colossal permittivity. *Acta Materialia*, **2019**, 164, 76-89	8.4	43
64	A first-principles study of Sc-decorated graphene with pyridinic-N defects for hydrogen storage. *International Journal of Hydrogen Energy*, **2017**, 42, 3106-3113	6.7	34
63	Ultrathin polymer film formation by collision-induced cross-linking of adsorbed organic molecules with hyperthermal protons. *Journal of the American Chemical Society*, **2004**, 126, 12336-42	16.4	34
62	First principles study of structural and electronic properties of cubic phase of ZrO2 and HfO2. *Physica B: Condensed Matter*, **2014**, 434, 7-13	2.8	33
61	Band gap engineering of FeS2 under biaxial strain: a first principles study. *Physical Chemistry Chemical Physics*, **2014**, 16, 24466-72	3.6	31
60	Strain engineering the magnetic states of vacancy-doped monolayer MoSe 2. *Journal of Alloys and Compounds*, **2015**, 635, 307-313	5.7	29
59	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	9.5	28
58	3d transitional-metal single atom catalysis toward hydrogen evolution reaction on MXenes supports. *International Journal of Hydrogen Energy*, **2020**, 45, 14396-14406	6.7	26

57	Effect of strain on the magnetic states of transition-metal atoms doped monolayer WS2. *Computational Materials Science*, **2016**, 117, 354-360	3.2	23
56	First-principles study on armchair AlN nanoribbons with different edge terminations. *Superlattices and Microstructures*, **2014**, 67, 40-46	2.8	22
55	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	3	21
54	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	2.3	20
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	8.9	20
52	Electronic and Magnetic Properties of Defected Monolayer WSe with Vacancies. *Nanoscale Research Letters*, **2019**, 14, 192	5	19
51	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	3.6	19
50	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	5.7	18
49	First-principles investigations of transition-metal doped bilayer WS *Physical Chemistry Chemical Physics*, **2016**, 18, 10152-7	3.6	17
48	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	3.2	17
47	Calcium decorated two dimensional carbon allotropes for hydrogen storage: A first-principles study. *Computational Materials Science*, **2016**, 124, 106-113	3.2	15
46	Cu Anchored Ti2NO2 as High Performance Electrocatalyst for Oxygen Evolution Reaction: A Density Functional Theory Study. *ChemCatChem*, **2020**, 12, 4059-4066	5.2	14
45	Edges of graphene and carbon nanotubes with high catalytic performance for the oxygen reduction reaction. *Physical Chemistry Chemical Physics*, **2017**, 19, 21003-21011	3.6	14
44	Improved catalytic performance of monolayer nano-triangles WS2 and MoS2 on HER by 3d metals doping. *Computational Materials Science*, **2019**, 159, 333-340	3.2	14
43	Asymmetric MXene/monolayer transition metal dichalcogenide heterostructures for functional applications. *Npj Computational Materials*, **2019**, 5,	10.9	13
42	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	3.8	13
41	High Curie temperature and carrier mobility of novel Fe, Co and Ni carbide MXenes. *Nanoscale*, **2020**, 12, 11627-11637	7.7	12
40	Two-dimensional intrinsic ferromagnetic half-metals: monolayers Mn3X4 (X = Te, Se, S). *Journal of Materials Science*, **2020**, 55, 7680-7690	4.3	12

39	First-Principles Study on the Stability and STM Image of Borophene. *Nanoscale Research Letters*, **2017**, 12, 514	5	11
38	Hybrid Polymer Membrane Functionalized PBO Fibers/Cyanate Esters Wave-Transparent Laminated Composites. *Advanced Fiber Materials*,1	10.9	10
37	Ordered double-M elements MXenes TiMC: Large in-plane stiffness and ferromagnetism. *Journal of Magnetism and Magnetic Materials*, **2019**, 486, 165280	2.8	9
36	Computing pKa Values with a Mixing Hamiltonian Quantum Mechanical/Molecular Mechanical Approach. *Journal of Chemical Theory and Computation*, **2013**, 9, 4257-65	6.4	9
35	Cleaving C□H bonds with hyperthermal H2: facile chemistry to cross-link organic molecules under low chemical- and energy-loads. *Green Chemistry*, **2014**, 16, 1316-1325	10	8
34	Exploring the catalytic activity of MXenes Mn+1CnO2 for hydrogen evolution. *Journal of Materials Science*, **2019**, 54, 11378-11389	4.3	7
33	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	3	7
32	Structural and electronic properties of conducting Cu nanowire encapsulated in semiconducting zigzag carbon nanotubes: A first-principles study. *Physica Status Solidi (B): Basic Research*, **2012**, 249, 1033-1038	1.3	7
31	First-principles investigation on the interface of transition metal dichalcogenide MX2 (M = Mo, W; X = S, Se) monolayer on Al2O3(0 0 0 1). *Computational Materials Science*, **2016**, 122, 118-125	3.2	7
30	Numerical simulation of lubrication performance on chevron textured surface under hydrodynamic lubrication. *Tribology International*, **2021**, 154, 106704	4.9	7
29	Electronic and magnetic properties of group-V TMDs monolayers with defects: A first-principles study. *Computational Materials Science*, **2020**, 176, 109540	3.2	6
28	Two-dimensional stable Fe-based ferromagnetic semiconductors: FeI and FeICl monolayers. *Physical Chemistry Chemical Physics*, **2020**, 22, 24506-24515	3.6	6
27	Pmma-XO (X´=´C, Si, Ge) monolayer as promising anchoring materials for lithium-sulfur battery: a first-principles study. *Nanotechnology*, **2019**, 30, 085405	3.4	6
26	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	8.4	6
25	A first-principles study on the electronic and magnetic properties of armchair SiC/AlN nanoribbons. *Journal of Alloys and Compounds*, **2014**, 586, 176-179	5.7	5
24	Dimethyl Disulfide on Cu(111): From Nondissociative to Dissociative Adsorption. *Journal of Physical Chemistry C*, **2013**, 117, 6587-6593	3.8	5
23	Ferromagnetic half-metal with high Curie temperature: Janus Mn2PAs monolayer. *Journal of Materials Science*, **2021**, 56, 13215-13226	4.3	5
22	First-principles study the single-layer transition metal trihalide CrXSe (X = Sn, Ge, Si) as monolayer ferromagnetic semiconductor. *Journal of Physics Condensed Matter*, **2020**, 32, 085801	1.8	4

21	First-Principles Study on the Electronic and Magnetic Properties of Zigzag AlN-SiC Nanoribbons. *Journal of Superconductivity and Novel Magnetism*, **2014**, 27, 1079-1082	1.5	4
20	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	3.8	4
19	Density Functional Theory Studies on the Adsorption of Methanethiol Molecule on Au(111) Surface at Different Coverage. *Acta Chimica Sinica*, **2013**, 71, 829	3.3	4
18	Magnetic semiconducting and strain-induced semiconducting–metallic transition in Cu-doped single-layer WSe2. *Journal of Materials Science*, **2019**, 54, 529-539	4.3	4
17	Revealing the Potential Crystal Structures of Earth-Abundant Nontoxic Photovoltaic CuBiI4. *Crystal Growth and Design*, **2021**, 21, 2850-2855	3.5	3
16	Room-temperature ferromagnetism in alkaline-earth-metal doped AlP: First-principle calculations. *Computational Materials Science*, **2018**, 142, 338-345	3.2	3
15	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	8.6	3
14	Self-assembled monolayers of CH3S from the adsorption of CH3SSCH3 on Au(111). *Physical Chemistry Chemical Physics*, **2014**, 16, 2533-41	3.6	2
13	Single transition metal atom anchored on VSe2 as electrocatalyst for nitrogen reduction reaction. *Applied Surface Science*, **2022**, 580, 152272	6.7	2
12	Stabilization and Metallic to Semiconducting Transition in 2D Boron Sheet. *Engineered Science*, **2018** ,	3.8	2
11	DID Code: A Bridge Connecting the Materials Genome Engineering Database with Inheritable Integrated Intelligent Manufacturing. *Engineering*, **2020**, 6, 612-620	9.7	1
10	DENSITY FUNCTIONAL THEORY STUDIES ON THE ADSORPTION OF 4-METHYLBENZENETHIOL AND 4-ETHYLBENZENETHIOL MOLECULES ON Au(111) SURFACE. *Surface Review and Letters*, **2014**, 21, 1450087	1.1	1
9	Tunable magnetic order in two-dimensional layered GdGe2. *Journal of Materials Chemistry C*, **2022**, 10, 1259-1269	7.1	1
8	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	6.7	1
7	Lattice distortion-enhanced superlubricity of (Mo, X)S (X = Al, Ti, Cr and V) with moiré superlattice. *Nanoscale*, **2021**, 13, 16234-16243	7.7	1
6	Response to comment on "Point defect structure of La-doped SrTiO3 ceramics with colossal permittivity" *Scripta Materialia*, **2021**, 190, 118-120	5.6	0
5	Robust Superlubricity and Moiré Lattice's Size Dependence on Friction between Graphdiyne Layers. *ACS Applied Materials & Interfaces*, **2021**, 13, 40901-40908	9.5	0
4	High-temperature ferromagnetism in monolayers MnGaX3 (X = Te, Se). *Journal of Magnetism and Magnetic Materials*, **2021**, 534, 168041	2.8	0

3	3-Fold-Periodic Size-Dependence in Electronic Properties of Monolayer-TMDC Nanotriangles. *Journal of Physical Chemistry Letters*, **2018**, 9, 1346-1352	6.4
2	Effects of intrinsic defects on methanthiol monolayers on Cu(111): a density functional theory study. *Journal of Chemical Physics*, **2013**, 138, 134708	3.9
1	Virtual voids method to generate low-density microporous carbon structures using quenched molecular dynamics simulation. *Carbon*, **2021**, 183, 438-448	10.4