

# Xiao-Li Fan

## List of Publications by Year in Descending Order

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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.

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	Tunable magnetic order in two-dimensional layered GdGe <sub>2</sub> . <i>Journal of Materials Chemistry C</i> , <b>2022</b> , 10, 1259-1269	7.1	1
73	Single transition metal atom anchored on VSe <sub>2</sub> as electrocatalyst for nitrogen reduction reaction. <i>Applied Surface Science</i> , <b>2022</b> , 580, 152272	6.7	2
72	Significantly improved interfacial properties and wave-transparent performance of PBO fibers/cyanate esters laminated composites via introducing a polydopamine/ZIF-8 hybrid membrane. <i>Composites Science and Technology</i> , <b>2022</b> , 223, 109426	8.6	3
71	Revealing the Potential Crystal Structures of Earth-Abundant Nontoxic Photovoltaic CuBi <sub>4</sub> . <i>Crystal Growth and Design</i> , <b>2021</b> , 21, 2850-2855	3.5	3
70	Ferromagnetic half-metal with high Curie temperature: Janus Mn <sub>2</sub> PAs monolayer. <i>Journal of Materials Science</i> , <b>2021</b> , 56, 13215-13226	4.3	5
69	Response to comment on point defect structure of La-doped SrTiO <sub>3</sub> ceramics with colossal permittivity. <i>Scripta Materialia</i> , <b>2021</b> , 190, 118-120	5.6	0
68	Numerical simulation of lubrication performance on chevron textured surface under hydrodynamic lubrication. <i>Tribology International</i> , <b>2021</b> , 154, 106704	4.9	7
67	Robust Superlubricity and Moiré Lattice's Size Dependence on Friction between Graphdiyne Layers. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2021</b> , 13, 40901-40908	9.5	0
66	High-temperature ferromagnetism in monolayers MnGaX <sub>3</sub> (X = Te, Se). <i>Journal of Magnetism and Magnetic Materials</i> , <b>2021</b> , 534, 168041	2.8	0
65	Virtual voids method to generate low-density microporous carbon structures using quenched molecular dynamics simulation. <i>Carbon</i> , <b>2021</b> , 183, 438-448	10.4	
64	Improving the comprehensive properties of PBO fibres/cyanate ester composites using a hyperbranched fluorine and epoxy containing PBO precursor. <i>Composites Part A: Applied Science and Manufacturing</i> , <b>2021</b> , 150, 106596	8.4	6
63	Calcium-doped ceria hybrid coating functionalized PBO fibers with excellent UV resistance and improved interfacial compatibility with cyanate ester resins. <i>Applied Surface Science</i> , <b>2021</b> , 569, 151124	6.7	1
62	Lattice distortion-enhanced superlubricity of (Mo, X)S <sub>2</sub> (X = Al, Ti, Cr and V) with moiré superlattice. <i>Nanoscale</i> , <b>2021</b> , 13, 16234-16243	7.7	1
61	Cu Anchored Ti <sub>2</sub> NO <sub>2</sub> as High Performance Electrocatalyst for Oxygen Evolution Reaction: A Density Functional Theory Study. <i>ChemCatChem</i> , <b>2020</b> , 12, 4059-4066	5.2	14
60	DID Code: A Bridge Connecting the Materials Genome Engineering Database with Inheritable Integrated Intelligent Manufacturing. <i>Engineering</i> , <b>2020</b> , 6, 612-620	9.7	1
59	First-principles study the single-layer transition metal trihalide CrXSe (X = Sn, Ge, Si) as monolayer ferromagnetic semiconductor. <i>Journal of Physics Condensed Matter</i> , <b>2020</b> , 32, 085801	1.8	4
58	Electronic and magnetic properties of group-V TMDs monolayers with defects: A first-principles study. <i>Computational Materials Science</i> , <b>2020</b> , 176, 109540	3.2	6

57	High Curie temperature and carrier mobility of novel Fe, Co and Ni carbide MXenes. <i>Nanoscale</i> , <b>2020</b> , 12, 11627-11637	7.7	12
56	Two-dimensional intrinsic ferromagnetic half-metals: monolayers Mn <sub>3</sub> X <sub>4</sub> (X = Te, Se, S). <i>Journal of Materials Science</i> , <b>2020</b> , 55, 7680-7690	4.3	12
55	3d transitional-metal single atom catalysis toward hydrogen evolution reaction on MXenes supports. <i>International Journal of Hydrogen Energy</i> , <b>2020</b> , 45, 14396-14406	6.7	26
54	Two-dimensional stable Fe-based ferromagnetic semiconductors: FeI and FeCl monolayers. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 24506-24515	3.6	6
53	Single Atoms on a Nitrogen-Doped Boron Phosphide Monolayer: A New Promising Bifunctional Electrocatalyst for ORR and OER. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2020</b> , 12, 52549-52559	9.5	28
52	Electronic and Magnetic Properties of Defected Monolayer WSe with Vacancies. <i>Nanoscale Research Letters</i> , <b>2019</b> , 14, 192	5	19
51	Exploring the catalytic activity of MXenes Mn <sub>n</sub> +1CnO <sub>2</sub> for hydrogen evolution. <i>Journal of Materials Science</i> , <b>2019</b> , 54, 11378-11389	4.3	7
50	Ordered double-M elements MXenes TiMC: Large in-plane stiffness and ferromagnetism. <i>Journal of Magnetism and Magnetic Materials</i> , <b>2019</b> , 486, 165280	2.8	9
49	Sc <sub>2</sub> CO <sub>2</sub> and Mn-doped Sc <sub>2</sub> CO <sub>2</sub> as gas sensor materials to NO and CO: A first-principles study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2019</b> , 111, 84-90	3	21
48	Asymmetric MXene/monolayer transition metal dichalcogenide heterostructures for functional applications. <i>Npj Computational Materials</i> , <b>2019</b> , 5,	10.9	13
47	Role of intrinsic dipole on photocatalytic water splitting for Janus MoSSe/nitrides heterostructure: A first-principles study. <i>Progress in Natural Science: Materials International</i> , <b>2019</b> , 29, 335-340	3.6	19
46	Magnetic semiconducting and strain-induced semiconducting-metallic transition in Cu-doped single-layer WSe <sub>2</sub> . <i>Journal of Materials Science</i> , <b>2019</b> , 54, 529-539	4.3	4
45	Improved catalytic performance of monolayer nano-triangles WS <sub>2</sub> and MoS <sub>2</sub> on HER by 3d metals doping. <i>Computational Materials Science</i> , <b>2019</b> , 159, 333-340	3.2	14
44	Point defect structure of La-doped SrTiO <sub>3</sub> ceramics with colossal permittivity. <i>Acta Materialia</i> , <b>2019</b> , 164, 76-89	8.4	43
43	Pmma-XO (X=C, Si, Ge) monolayer as promising anchoring materials for lithium-sulfur battery: a first-principles study. <i>Nanotechnology</i> , <b>2019</b> , 30, 085405	3.4	6
42	3-Fold-Periodic Size-Dependence in Electronic Properties of Monolayer-TMDC Nanotriangles. <i>Journal of Physical Chemistry Letters</i> , <b>2018</b> , 9, 1346-1352	6.4	
41	Laminated Hybrid Junction of Sulfur-Doped TiO and a Carbon Substrate Derived from TiC MXenes: Toward Highly Visible Light-Driven Photocatalytic Hydrogen Evolution. <i>Advanced Science</i> , <b>2018</b> , 5, 1700870	12.6	108
40	Enhanced gas-sensing performance of graphene by doping transition metal atoms: A first-principles study. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , <b>2018</b> , 382, 2965-2973	2.3	20

39	MXene Nanofibers as Highly Active Catalysts for Hydrogen Evolution Reaction. <i>ACS Sustainable Chemistry and Engineering</i> , <b>2018</b> , 6, 8976-8982	8.3	103
38	Stabilization and Metallic to Semiconducting Transition in 2D Boron Sheet. <i>Engineered Science</i> , <b>2018</b> , ,	3.8	2
37	Room-temperature ferromagnetism in alkaline-earth-metal doped ALP: First-principle calculations. <i>Computational Materials Science</i> , <b>2018</b> , 142, 338-345	3.2	3
36	Ferroelectric-Enhanced Polysulfide Trapping for Lithium-Sulfur Battery Improvement. <i>Advanced Materials</i> , <b>2017</b> , 29, 1604724	24	124
35	Nanopolygons of Monolayer MS: Best Morphology and Size for HER Catalysis. <i>Nano Letters</i> , <b>2017</b> , 17, 368-376	11.5	71
34	A first-principles study of Sc-decorated graphene with pyridinic-N defects for hydrogen storage. <i>International Journal of Hydrogen Energy</i> , <b>2017</b> , 42, 3106-3113	6.7	34
33	First-Principles Study on the Stability and STM Image of Borophene. <i>Nanoscale Research Letters</i> , <b>2017</b> , 12, 514	5	11
32	Edges of graphene and carbon nanotubes with high catalytic performance for the oxygen reduction reaction. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 21003-21011	3.6	14
31	Ferromagnetism in Transitional Metal-Doped MoS <sub>2</sub> Monolayer. <i>Nanoscale Research Letters</i> , <b>2016</b> , 11, 154	5	75
30	Catalytic Activity of MS <sub>2</sub> Monolayer for Electrochemical Hydrogen Evolution. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 1623-1632	3.8	67
29	First-principles investigations of transition-metal doped bilayer WS <sub>2</sub> . <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 10152-7	3.6	17
28	Effect of strain on the magnetic states of transition-metal atoms doped monolayer WS <sub>2</sub> . <i>Computational Materials Science</i> , <b>2016</b> , 117, 354-360	3.2	23
27	First-principles investigation on the interface of transition metal dichalcogenide MX <sub>2</sub> (M = Mo, W; X = S, Se) monolayer on Al <sub>2</sub> O <sub>3</sub> (0 0 1). <i>Computational Materials Science</i> , <b>2016</b> , 122, 118-125	3.2	7
26	Calcium decorated two dimensional carbon allotropes for hydrogen storage: A first-principles study. <i>Computational Materials Science</i> , <b>2016</b> , 124, 106-113	3.2	15
25	Uncovering the Veil of the Degradation in Perovskite CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> upon Humidity Exposure: A First-Principles Study. <i>Journal of Physical Chemistry Letters</i> , <b>2015</b> , 6, 3289-3295	6.4	147
24	Composition Directed Generation of Reactive Oxygen Species in Irradiated Mixed Metal Sulfides Correlated with Their Photocatalytic Activities. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2015</b> , 7, 16440-9	9.5	52
23	Strain engineering the magnetic states of vacancy-doped monolayer MoSe <sub>2</sub> . <i>Journal of Alloys and Compounds</i> , <b>2015</b> , 635, 307-313	5.7	29
22	Increasing the band gap of FeS <sub>2</sub> by alloying with Zn and applying biaxial strain: A first-principles study. <i>Journal of Alloys and Compounds</i> , <b>2015</b> , 629, 43-48	5.7	18

21	Room-temperature preparation of trisilver-copper-sulfide/polymer based heterojunction thin film for solar cell application. <i>Journal of Power Sources</i> , <b>2015</b> , 280, 313-319	8.9	20
20	First-principles study on armchair AlN nanoribbons with different edge terminations. <i>Superlattices and Microstructures</i> , <b>2014</b> , 67, 40-46	2.8	22
19	A first-principles study on the electronic and magnetic properties of armchair SiC/AlN nanoribbons. <i>Journal of Alloys and Compounds</i> , <b>2014</b> , 586, 176-179	5.7	5
18	Cleaving C≡I bonds with hyperthermal H <sub>2</sub> : facile chemistry to cross-link organic molecules under low chemical- and energy-loads. <i>Green Chemistry</i> , <b>2014</b> , 16, 1316-1325	10	8
17	First principles study of structural and electronic properties of cubic phase of ZrO <sub>2</sub> and HfO <sub>2</sub> . <i>Physica B: Condensed Matter</i> , <b>2014</b> , 434, 7-13	2.8	33
16	First-Principles Study on the Electronic and Magnetic Properties of Zigzag AlN-SiC Nanoribbons. <i>Journal of Superconductivity and Novel Magnetism</i> , <b>2014</b> , 27, 1079-1082	1.5	4
15	Site-specific catalytic activity in exfoliated MoS <sub>2</sub> single-layer polytypes for hydrogen evolution: basal plane and edges. <i>Journal of Materials Chemistry A</i> , <b>2014</b> , 2, 20545-20551	13	127
14	Self-assembled monolayers of CH <sub>3</sub> S from the adsorption of CH <sub>3</sub> SSCH <sub>3</sub> on Au(111). <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 2533-41	3.6	2
13	Band gap engineering of FeS <sub>2</sub> under biaxial strain: a first principles study. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 24466-72	3.6	31
12	Tuning the electronic properties of half- and full-hydrogenated germanene by chlorination and hydroxylation: A first-principles study. <i>Computational Materials Science</i> , <b>2014</b> , 92, 244-252	3.2	17
11	Density functional theory study of the adsorption of methanethiol on Au(111): Role of gold adatoms. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2014</b> , 59, 248-253	3	7
10	DENSITY FUNCTIONAL THEORY STUDIES ON THE ADSORPTION OF 4-METHYLBENZENETHIOL AND 4-ETHYLBENZENETHIOL MOLECULES ON Au(111) SURFACE. <i>Surface Review and Letters</i> , <b>2014</b> , 21, 1450087	1.1	1
9	Computing pKa Values with a Mixing Hamiltonian Quantum Mechanical/Molecular Mechanical Approach. <i>Journal of Chemical Theory and Computation</i> , <b>2013</b> , 9, 4257-65	6.4	9
8	Dimethyl Disulfide on Cu(111): From Nondissociative to Dissociative Adsorption. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 6587-6593	3.8	5
7	Effects of intrinsic defects on methanethiol monolayers on Cu(111): a density functional theory study. <i>Journal of Chemical Physics</i> , <b>2013</b> , 138, 134708	3.9	
6	Density Functional Theory Studies on the Adsorption of Methanethiol Molecule on Au(111) Surface at Different Coverage. <i>Acta Chimica Sinica</i> , <b>2013</b> , 71, 829	3.3	4
5	From Nondissociative to Dissociative Adsorption of Benzene-thiol on Au(111): A Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 1002-1011	3.8	13
4	Effects of Intrinsic Surface Defects on Thiophenol Self-Assembly on Au(111): Surface Structures and Reaction Mechanisms. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 19909-19917	3.8	4

- 3 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<sup>1,3,7</sup>
- 2 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
- 1 Hybrid Polymer Membrane Functionalized PBO Fibers/Cyanate Esters Wave-Transparent Laminated Composites. *Advanced Fiber Materials*, 1 10.9 10