

# Pei-Fei Liu

## List of Publications by Citations

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132  
ext. papers

4,518  
ext. citations

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avg, IF

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L-index

#	Paper	IF	Citations
115	Homogeneously dispersed multimetal oxygen-evolving catalysts. <i>Science</i> , <b>2016</b> , 352, 333-7	33.3	1459
114	Cobalt Covalent Doping in MoS to Induce Bifunctionality of Overall Water Splitting. <i>Advanced Materials</i> , <b>2018</b> , 30, e1801450	24	273
113	Ba <sub>6</sub> Zn <sub>7</sub> Ga <sub>2</sub> S <sub>16</sub> : A Wide Band Gap Sulfide with Phase-Matchable Infrared NLO Properties. <i>Chemistry of Materials</i> , <b>2017</b> , 29, 5259-5266	9.6	72
112	Monolayer SnP: an excellent p-type thermoelectric material. <i>Nanoscale</i> , <b>2019</b> , 11, 19923-19932	7.7	66
111	Strong IR NLO Material Ba <sub>4</sub> MGa <sub>4</sub> Se <sub>10</sub> Cl <sub>2</sub> : Highly Improved Laser Damage Threshold via Dual Ion Substitution Synergy. <i>Advanced Optical Materials</i> , <b>2015</b> , 3, 957-966	8.1	50
110	Hexagonal TiB monolayer: a promising anode material offering high rate capability for Li-ion and Na-ion batteries. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 22168-22178	3.6	49
109	First-principles calculations of the ultralow thermal conductivity in two-dimensional group-IV selenides. <i>Physical Review B</i> , <b>2018</b> , 98,	3.3	48
108	Tetragonal and trigonal MoB monolayers: two new low-dimensional materials for Li-ion and Na-ion batteries. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 5178-5188	3.6	45
107	Application of first-principles theory in ferrite phases of cemented paste backfill. <i>Minerals Engineering</i> , <b>2019</b> , 133, 47-51	4.9	39
106	Experimental and theoretical studies on the NLO properties of two quaternary non-centrosymmetric chalcogenides: BaAgGeS and BaAgSnS. <i>Dalton Transactions</i> , <b>2018</b> , 47, 429-437	4.3	38
105	Two Phosphates: Noncentrosymmetric CsMg(PO) and Centrosymmetric CsMgZn(PO). <i>Inorganic Chemistry</i> , <b>2017</b> , 56, 845-851	5.1	37
104	Monolayer Zr <sub>2</sub> B <sub>2</sub> : A promising two-dimensional anode material for Li-ion batteries. <i>Applied Surface Science</i> , <b>2019</b> , 480, 448-453	6.7	37
103	Understanding Cement Hydration of Cemented Paste Backfill: DFT Study of Water Adsorption on Tricalcium Silicate (111) Surface. <i>Minerals (Basel, Switzerland)</i> , <b>2019</b> , 9, 202	2.4	37
102	Salt-Inclusion Chalcogenide [Ba <sub>4</sub> Cl <sub>2</sub> ][ZnGa <sub>4</sub> S <sub>10</sub> ]: Rational Design of an IR Nonlinear Optical Material with Superior Comprehensive Performance Derived from AgGaS <sub>2</sub> . <i>Chemistry of Materials</i> , <b>2020</b> , 32, 8012-8019	9.6	34
101	Sr <sub>5</sub> ZnGa <sub>6</sub> S <sub>15</sub> : a new quaternary non-centrosymmetric semiconductor with a 3D framework structure displaying excellent nonlinear optical performance. <i>Inorganic Chemistry Frontiers</i> , <b>2018</b> , 5, 1458-1462 <sup>6,8,33</sup>	6.8	33
100	Electron-Rich Ruthenium on Nitrogen-Doped Carbons Promoting Levulinic Acid Hydrogenation to $\gamma$ -Valerolactone: Effect of Metal Support Interaction. <i>ACS Sustainable Chemistry and Engineering</i> , <b>2019</b> , 7, 16501-16510	8.3	32
99	Pressure-induced irreversible metallization accompanying the phase transitions in Sb <sub>2</sub> S <sub>3</sub> . <i>Physical Review B</i> , <b>2018</b> , 97,	3.3	32

98	Hexagonal M <sub>2</sub> C <sub>3</sub> (M = As, Sb, and Bi) monolayers: new functional materials with desirable band gaps and ultrahigh carrier mobility. <i>Journal of Materials Chemistry C</i> , <b>2018</b> , 6, 12689-12697	7.1	30
97	Tailored synthesis of nonlinear optical quaternary chalcogenides: BaGeS <sub>2</sub> Cl, BaSiSeCl and BaGeSeCl. <i>Dalton Transactions</i> , <b>2017</b> , 46, 2715-2721	4.3	29
96	Prediction of phonon-mediated superconductivity in two-dimensional Mo <sub>2</sub> B <sub>2</sub> . <i>Journal of Materials Chemistry C</i> , <b>2019</b> , 7, 2589-2595	7.1	29
95	First-principles study of thermal transport properties in the two- and three-dimensional forms of BiOSe. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 10931-10938	3.6	27
94	Evidence for Ferroelectricity of All-Inorganic Perovskite CsPbBr <sub>3</sub> Quantum Dots. <i>Journal of the American Chemical Society</i> , <b>2020</b> , 142, 3316-3320	16.4	27
93	Ba <sub>6</sub> Li <sub>2</sub> CdSn <sub>4</sub> S <sub>16</sub> : lithium substitution simultaneously enhances band gap and SHG intensity. <i>Journal of Materials Chemistry C</i> , <b>2017</b> , 5, 7067-7074	7.1	27
92	Vanadium sulfide sub-microspheres: A new near-infrared-driven photocatalyst. <i>Journal of Colloid and Interface Science</i> , <b>2017</b> , 498, 442-448	9.3	26
91	Ultralow thermal conductivity from transverse acoustic phonon suppression in distorted crystalline $\beta$ -MgAgSb. <i>Nature Communications</i> , <b>2020</b> , 11, 942	17.4	26
90	Superconductivity in two-dimensional phosphorus carbide (EPC). <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 12362-12367	3.6	26
89	High Thermoelectric Performance of New Two-Dimensional IV <sup>VI</sup> Compounds: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , <b>2020</b> , 124, 1812-1819	3.8	25
88	Two-dimensional hexagonal M <sub>3</sub> C <sub>2</sub> (M = Zn, Cd and Hg) monolayers: novel quantum spin Hall insulators and Dirac cone materials. <i>Journal of Materials Chemistry C</i> , <b>2017</b> , 5, 9181-9187	7.1	24
87	A graphene-like MgN monolayer: high stability, desirable direct band gap and promising carrier mobility. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 30379-30384	3.6	24
86	The effect of indium substitution on the structure and NLO properties of Ba <sub>6</sub> Cs <sub>2</sub> Ga <sub>10</sub> Se <sub>20</sub> Cl <sub>4</sub> . <i>Inorganic Chemistry Frontiers</i> , <b>2016</b> , 3, 952-958	6.8	23
85	Structure disorder of graphitic carbon nitride induced by liquid-assisted grinding for enhanced photocatalytic conversion. <i>RSC Advances</i> , <b>2014</b> , 4, 10676-10679	3.7	23
84	Two-dimensional spin-valley-coupled Dirac semimetals in functionalized SbAs monolayers. <i>Materials Horizons</i> , <b>2019</b> , 6, 781-787	14.4	21
83	First-principles calculations of thermal transport properties in MoS/MoSe bilayer heterostructure. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 10442-10448	3.6	21
82	Enhanced adsorption properties of bimetallic RuCo catalyst for the hydrodeoxygenation of phenolic compounds and raw lignin-oil. <i>Chemical Engineering Science</i> , <b>2020</b> , 227, 115920	4.4	20
81	Solvent-free hydrodeoxygenation of bio-lipids into renewable alkanes over NiW bimetallic catalyst under mild conditions. <i>Applied Catalysis B: Environmental</i> , <b>2020</b> , 269, 118718	21.8	20

80	New quantum spin Hall insulator in two-dimensional MoS <sub>2</sub> with periodically distributed pores. <i>Nanoscale</i> , <b>2016</b> , 8, 4915-21	7.7	19
79	Theoretical dissection of superconductivity in two-dimensional honeycomb borophene oxide B <sub>2</sub> O crystal with a high stability. <i>Npj Computational Materials</i> , <b>2020</b> , 6,	10.9	18
78	Controlled Synthesis of Bifunctional NiCo <sub>2</sub> O <sub>4</sub> @FeNi LDH Core/Shell Nanoarray Air Electrodes for Rechargeable Zinc-Air Batteries. <i>ACS Sustainable Chemistry and Engineering</i> , <b>2020</b> , 8, 11079-11087	8.3	17
77	Superconductivity in predicted two dimensional XB <sub>6</sub> (X = Ga, In). <i>Journal of Materials Chemistry C</i> , <b>2020</b> , 8, 1704-1714	7.1	17
76	Thermoelectric Properties of Hexagonal M <sub>2</sub> Te <sub>3</sub> (M = As, Sb, and Bi) Monolayers from First-Principles Calculations. <i>Nanomaterials</i> , <b>2019</b> , 9,	5.4	16
75	Pressure-induced metallization in MoSe under different pressure conditions.. <i>RSC Advances</i> , <b>2019</b> , 9, 5794-5803	3.7	16
74	Electronic structure and photoluminescence of Dy <sup>3+</sup> single-doped and Dy <sup>3+</sup> /Tm <sup>3+</sup> co-doped NaBi(WO <sub>4</sub> ) <sub>2</sub> phosphors. <i>Optical Materials</i> , <b>2019</b> , 88, 534-539	3.3	15
73	Hydrodeoxygenation of phenolic compounds and raw lignin-oil over bimetallic RuNi catalyst: An experimental and modeling study focusing on adsorption properties. <i>Fuel</i> , <b>2020</b> , 281, 118758	7.1	14
72	Emergence of superconductivity in a Dirac nodal-line Cu <sub>2</sub> Si monolayer: ab initio calculations. <i>Journal of Materials Chemistry C</i> , <b>2019</b> , 7, 10926-10932	7.1	13
71	Trap distribution and photo-stimulated luminescence in LaSrAl <sub>3</sub> O <sub>7</sub> :Eu <sup>2+</sup> long-lasting phosphors for optical data storage. <i>Journal of the American Ceramic Society</i> , <b>2020</b> , 103, 315-323	3.8	13
70	Novel structures of two-dimensional tungsten boride and their superconductivity. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 15327-15338	3.6	12
69	Quaternary semiconductor BaZnGaS featuring unique one-dimensional chains and exhibiting desirable yellow emission. <i>Chemical Communications</i> , <b>2019</b> , 55, 7942-7945	5.8	12
68	Synthesis, crystal and electronic structure, and optical property of the pentanary chalcogenide Ba <sub>3</sub> K <sub>2</sub> Sb <sub>4</sub> S <sub>9</sub> Cl. <i>Journal of Solid State Chemistry</i> , <b>2015</b> , 232, 37-41	3.3	12
67	First-principles study of superconductivity in the two- and three-dimensional forms of PbTiSe <sub>2</sub> : Suppressed charge density wave in 1T <sub>1</sub> Te <sub>2</sub> . <i>Physical Review B</i> , <b>2018</b> , 98,	3.3	12
66	Modifying Disordered Sites with Rational Cations to Regulate Band-Gaps and Second Harmonic Generation Responses Markedly: Ba <sub>6</sub> Li <sub>2</sub> ZnSn <sub>4</sub> S <sub>16</sub> vs Ba <sub>6</sub> Ag <sub>2</sub> ZnSn <sub>4</sub> S <sub>16</sub> vs Ba <sub>6</sub> Li <sub>2.67</sub> Sn <sub>4.33</sub> S <sub>16</sub> . <i>Crystal Growth and Design</i> , <b>2018</b> , 18, 5609-5616	3.5	12
65	Syntheses and characterization of three new sulfides with large band gaps: acentric BaGaSnS, centric BaSnS and BaSnS. <i>Dalton Transactions</i> , <b>2017</b> , 46, 14771-14778	4.3	12
64	Two-dimensional hydrogenated molybdenum and tungsten dinitrides MNH (M = Mo, W) as novel quantum spin hall insulators with high stability. <i>Nanoscale</i> , <b>2017</b> , 9, 1007-1013	7.7	11
63	Effects of Impurity Doping on the Luminescence Performance of Mn-Doped Aluminates with the Magnetoplumbite-Type Structure for Plant Cultivation. <i>Materials</i> , <b>2018</b> , 12,	3.5	11

62	Li <sub>3</sub> Cs <sub>2</sub> M <sub>2</sub> B <sub>3</sub> P <sub>6</sub> O <sub>24</sub> (M = Pb, Sr): borophosphates with double six-membered ring of [BP <sub>2</sub> O <sub>8</sub> ](3.). <i>Dalton Transactions</i> , <b>2016</b> , 45, 7124-30	4.3	11
61	Syntheses, structures, physical and electronic properties of quaternary semiconductors: Cs[RE <sub>9</sub> Cd <sub>4</sub> Se <sub>18</sub> ] (RE = Tb-Tm). <i>Dalton Transactions</i> , <b>2016</b> , 45, 5775-82	4.3	11
60	Syntheses, structures, and properties of sulfides constructed by SbS <sub>4</sub> teeter-totter polyhedra: Ba <sub>3</sub> La <sub>4</sub> Ga <sub>2</sub> Sb <sub>2</sub> S <sub>15</sub> and BaLa <sub>3</sub> GaSb <sub>2</sub> S <sub>10</sub> . <i>Inorganic Chemistry Frontiers</i> , <b>2017</b> , 4, 123-130	6.8	10
59	The roles of Yb-substitution on thermoelectric properties of In <sub>4</sub> Yb <sub>3</sub> Se <sub>3</sub> . <i>Acta Materialia</i> , <b>2015</b> , 101, 16-218.4	10	10
58	Pollution levels, composition characteristics and sources of atmospheric PM in a rural area of the North China Plain during winter. <i>Journal of Environmental Sciences</i> , <b>2020</b> , 95, 172-182	6.4	10
57	High-pressure structural phase transition and metallization in Ga <sub>2</sub> S <sub>3</sub> under non-hydrostatic and hydrostatic conditions up to 36.4 GPa. <i>Journal of Materials Chemistry C</i> , <b>2021</b> , 9, 2912-2918	7.1	10
56	Multidirectional Intrinsic Piezoelectricity of 2D Metal ChalcogenDiphosphate ABP <sub>2</sub> X <sub>6</sub> Monolayers. <i>Physica Status Solidi - Rapid Research Letters</i> , <b>2020</b> , 14, 2000321	2.5	9
55	Ternary multicomponent Ba/Mg/Si compounds with inherent bonding hierarchy and rattling Ba atoms toward low lattice thermal conductivity. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 18556-18561	2.6	9
54	Band-aligned C <sub>3</sub> N <sub>4</sub> S <sub>3</sub> x/2 stabilizes CdS/CuInGaS <sub>2</sub> photocathodes for efficient water reduction. <i>Journal of Materials Chemistry A</i> , <b>2017</b> , 5, 3167-3171	13	8
53	Phase Transition and Metallization of Orpiment by Raman Spectroscopy, Electrical Conductivity and Theoretical Calculation under High Pressure. <i>Materials</i> , <b>2019</b> , 12,	3.5	8
52	(Cs <sub>6</sub> Cl) <sub>6</sub> Cs <sub>3</sub> [Ga <sub>5</sub> Se <sub>9</sub> ]: A Unique Long Period-Stacking Structure of Layers Made from Ga <sub>2</sub> Se <sub>6</sub> Dimers via Cis or Trans Intralayer Linking. <i>Inorganic Chemistry</i> , <b>2016</b> , 55, 1014-6	5.1	8
51	Face-centered cubic MoS <sub>2</sub> : a novel superconducting three-dimensional crystal more stable than layered T-MoS <sub>2</sub> . <i>Journal of Materials Chemistry C</i> , <b>2018</b> , 6, 6046-6051	7.1	8
50	Topological and superconducting properties in YD <sub>3</sub> (D=In, Sn, Tl, Pb). <i>Physical Review Materials</i> , <b>2019</b> , 3,	3.2	8
49	Solid-State Preparation, Structural Characterization, Physical Properties, and Theoretical Studies of a Series of Novel Rare-Earth Metal Chalcogenides with Unprecedented Closed-Cavities. <i>Crystal Growth and Design</i> , <b>2019</b> , 19, 444-452	3.5	8
48	Centrosymmetric to noncentrosymmetric structural transformation of new quaternary selenides induced by isolated dimeric [Sn <sub>2</sub> Se <sub>4</sub> ] units: from Ba <sub>8</sub> Ga <sub>2</sub> Sn <sub>7</sub> Se <sub>18</sub> to Ba <sub>10</sub> Ga <sub>2</sub> Sn <sub>9</sub> Se <sub>22</sub> . <i>RSC Advances</i> , <b>2017</b> , 7, 8082-8089	3.7	7
47	Synthesis and characterization of mixed alkali borophosphate with a new 1D chain: Li <sub>3</sub> Cs <sub>2</sub> BP <sub>4</sub> O <sub>14</sub> . <i>Inorganica Chimica Acta</i> , <b>2017</b> , 466, 174-179	2.7	7
46	CsBi <sub>4</sub> Te <sub>6</sub> : a new facile synthetic method and mid-temperature thermoelectric performance. <i>Dalton Transactions</i> , <b>2016</b> , 45, 11931-4	4.3	7
45	Theoretical Study of the Electronic, Magnetic, Mechanical and Thermodynamic Properties of the Spin Gapless Semiconductor CoFeMnSi. <i>Crystals</i> , <b>2019</b> , 9, 678	2.3	7

44	Benzoquinone-bridged Co complexes with different magnetic anisotropy induced by solvent molecules. <i>Dalton Transactions</i> , <b>2017</b> , 46, 3435-3437	4.3	6
43	Lattice vibrational modes and phonon thermal conductivity of single-layer GaGeTe. <i>Journal of Materiomics</i> , <b>2020</b> , 6, 723-728	6.7	6
42	Significant enhancement of the thermoelectric properties of CaP3 through reducing the dimensionality. <i>Materials Advances</i> , <b>2020</b> , 1, 3322-3332	3.3	6
41	First-principles prediction of ideal type-II Weyl phonons in wurtzite ZnSe. <i>Physical Review B</i> , <b>2021</b> , 103,	3.3	6
40	A3Mn2Sb3S8 (A = K and Rb): a new type of multifunctional infrared nonlinear optical material based on unique three-dimensional open frameworks. <i>Inorganic Chemistry Frontiers</i> , <b>2021</b> , 8, 2835-2843	6.8	6
39	Quadruple-layer group-IV tellurides: low thermal conductivity and high performance two-dimensional thermoelectric materials. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 6388-6396	3.6	6
38	Square transition-metal carbides MC (M = Mo, W) as stable two-dimensional Dirac cone materials. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 732-737	3.6	6
37	Characterization of the pressure-induced phase transition of metallization for MoTe2 under hydrostatic and non-hydrostatic conditions. <i>AIP Advances</i> , <b>2019</b> , 9, 065104	1.5	5
36	Electron-phonon coupling superconductivity in two-dimensional orthorhombic MB6 (M=Mg,Ca,Ti,Y) and hexagonal MB6 (M=Mg,Ca,Sc,Ti). <i>Physical Review Materials</i> , <b>2020</b> , 4,	3.2	5
35	Dual regulation both intrinsic activity and mass transport for self-supported electrodes using in anion exchange membrane water electrolysis. <i>Chemical Engineering Journal</i> , <b>2021</b> , 431, 133942	14.7	5
34	Ultrathin Hematite Photoanode with Gradient Ti Doping. <i>Research</i> , <b>2020</b> , 2020, 5473217	7.8	5
33	First-principles investigation on the transport properties of quaternary CoFeRGa (R = Ti, V, Cr, Mn, Cu, and Nb) Heusler compounds. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 23185-23194	3.6	5
32	Syntheses of six and twelve membered borophosphate ring structure with nonlinear optical activity. <i>Journal of Solid State Chemistry</i> , <b>2016</b> , 243, 259-266	3.3	5
31	Ba10Zn7M6Q26: Two New Mid-infrared Nonlinear Optical Crystals with T2 Supertetrahedron 3D Framework. <i>Crystal Growth and Design</i> , <b>2019</b> , 19, 1190-1197	3.5	5
30	Surface-structure sensitive chemical diffusivity and reactivity of CO adsorbates on noble metal electrocatalysts. <i>Applied Catalysis B: Environmental</i> , <b>2021</b> , 281, 119522	21.8	5
29	Amino Acid Ionic Liquids Catalyzed d-Glucosamine into Pyrazine Derivatives: Insight from NMR Spectroscopy. <i>Journal of Agricultural and Food Chemistry</i> , <b>2021</b> , 69, 2403-2411	5.7	5
28	Understanding of transition metal (Ru, W) doping into Nb for improved thermodynamic stability and hydrogen permeability: density functional theory calculations. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 17538-17545	3.6	4
27	Complete spin gapless semiconductivity in equiatomic quaternary Heusler material TiZrMnAl. <i>Journal of Magnetism and Magnetic Materials</i> , <b>2020</b> , 508, 166880	2.8	4



26	Synthesis of well-defined functional crystals by high temperature gas-phase reactions. <i>Science Bulletin</i> , <b>2014</b> , 59, 2135-2143		4
25	Effects of structure and electronic properties of spinel ferrites on their emissivity in middle and short wavebands. <i>Journal of Solid State Chemistry</i> , <b>2020</b> , 282, 121089	3.3	4
24	Correlation between microstructure and dissolution property of magnesium hydroxide synthesized via magnesia hydroxylation: Effect of hydration agents. <i>Journal of Cleaner Production</i> , <b>2020</b> , 249, 119371 <sup>10.3</sup>		4
23	Prediction of superconductivity and topological aspects in single-layer Bi <sub>2</sub> Pd. <i>Physical Review B</i> , <b>2020</b> , 102,	3.3	4
22	Theoretical insights into heterogeneous single-atom Fe <sub>1</sub> catalysts supported by graphene-based substrates for water splitting. <i>Applied Surface Science</i> , <b>2021</b> , 540, 148245	6.7	4
21	Charge density wave and pressure-dependent superconductivity in the kagome metal CsV <sub>3</sub> Sb <sub>5</sub> : A first-principles study. <i>Physical Review B</i> , <b>2022</b> , 105,	3.3	3
20	The effect of CuFe <sub>2</sub> O <sub>4</sub> ferrite phase evolution on 35 μm waveband emissivity. <i>Ceramics International</i> , <b>2020</b> , 46, 7694-7702	5.1	3
19	Beyond the Limit of Goldschmidt Tolerance Factor: Crystal Surface Engineering to Boost the Phase Stability of Formamidinium-Only Hybrid Inorganic/Organic Perovskites. <i>Solar Rrl</i> , <b>2021</b> , 5, 2100188 <sup>7.1</sup>		3
18	Atomically Dispersed Cobalt in Core-Shell Carbon Nanofiber Membranes as Super-Flexible Freestanding Air-electrodes for Wearable Zn-air Batteries. <i>Energy Storage Materials</i> , <b>2022</b> , 47, 365-365	19.4	2
17	Phonon transport in Zintl Ba <sub>2</sub> ZnAs <sub>2</sub> and Ba <sub>2</sub> ZnSb <sub>2</sub> : A first-principles study. <i>Materials Science in Semiconductor Processing</i> , <b>2022</b> , 141, 106446	4.3	2
16	Thermoelectric Properties of Hexagonal WN from First-Principles Calculations. <i>ES Energy &amp; Environments</i> , <b>2018</b> ,	2.9	2
15	A new type of novel salt-inclusion chalcogenide with ultralow thermal conductivity. <i>Chemical Communications</i> , <b>2020</b> , 56, 15149-15152	5.8	2
14	Role of the Interfacial Effect between the Substrate and Co(OH) <sub>2</sub> Layer in Electrochemical Oxygen Evolution. <i>ACS Applied Energy Materials</i> , <b>2021</b> , 4, 9487-9497	6.1	2
13	Significant enhancement of VOCs conversion by facile mechanochemistry coupled MnO <sub>2</sub> modified fly ash: Mechanism and application. <i>Fuel</i> , <b>2021</b> , 304, 121443	7.1	2
12	Computational Study of the Curvature-Promoted Anchoring of Transition Metals for Water Splitting.. <i>Nanomaterials</i> , <b>2021</b> , 11,	5.4	1
11	Structural, electronic and optical properties of S-doped, Sc-doped and Sc <sub>3</sub> co-doped anatase TiO <sub>2</sub> : a DFT + U calculation. <i>European Physical Journal B</i> , <b>2020</b> , 93, 1	1.2	1
10	Novel 2D PC 5 with a Dirac Cone and Edge-Size Dependence. <i>Physica Status Solidi - Rapid Research Letters</i> , 2100203	2.5	1
9	Ba <sub>3</sub> [LiSbS <sub>2</sub> (S <sub>2</sub> ) <sub>2</sub> Cl <sub>2</sub> ]: The first zero-dimensional (0D) lithium metal thioantimonate featuring molecular anions of [LiSbS <sub>2</sub> (S <sub>2</sub> ) <sub>2</sub> Cl <sub>2</sub> ] <sup>6-</sup> <i>Journal of Solid State Chemistry</i> , <b>2021</b> , 294, 121873	3.3	1

8	Ultralow thermal conductivity in the quaternary semiconducting chalcogenide Cs <sub>4</sub> [Ho <sub>26</sub> Cd <sub>7</sub> Se <sub>48</sub> ] with an unprecedented closed cavity architecture. <i>Inorganic Chemistry Frontiers</i> , <b>2021</b> , 8, 1049-1055	6.8	1
7	Structural diversities in centrosymmetric LaSCLaSCL[SbS] and non-centrosymmetric LnSCL[SbS] (Ln = La and Ce): syntheses, crystal and electronic structures, and optical properties. <i>Dalton Transactions</i> , <b>2021</b> , 50, 2075-2082	4.3	1
6	Hydrophobic 1-octadecanethiol functionalized copper catalyst promotes robust high-current CO <sub>2</sub> gas-diffusion electrolysis. <i>Nano Research</i> , 1	10	1
5	A novel Mn-activated layered oxide-fluoride perovskite-type KNaMoOF red phosphor for wide gamut warm white light-emitting diode backlights. <i>Dalton Transactions</i> , <b>2021</b> , 50, 11189-11196	4.3	1
4	Topological Superconductivity in Rashba Spin-Orbital Coupling Suppressed Monolayer $\beta$ Bi <sub>2</sub> Pd. <i>Materials Today Physics</i> , <b>2022</b> , 100674	8	1
3	From Cc to P63mc: Structural Variation in La <sub>3</sub> S <sub>2</sub> Cl <sub>2</sub> [SbS <sub>3</sub> ] and La <sub>3</sub> OSCl <sub>2</sub> [SbS <sub>3</sub> ] Induced by the Isovalent Anion Substitution. <i>Crystal Growth and Design</i> , <b>2022</b> , 22, 1437-1444	3.5	0
2	Installation of high-valence tungsten in MIL-125(Ti) for boosted photocatalytic hydrogen evolution. <i>Science China Materials</i> , <b>2022</b> , 65, 1237-1244	7.1	0
1	First-principles study of electronic structure and superconductivity of PbTa <sub>2</sub> Se. <i>Materials Research Express</i> , <b>2019</b> , 6, 046001	1.7	