Lijun Zhang

List of Publications by Year
in descending order

166 papers	16,383 citations	23567 58 h-index	15732 125 g-index
169 all docs	169 docs citations	169 times ranked	15920 citing authors

#	Article	IF	Citations
1	Efficient and stable emission of warm-white light from lead-free halide double perovskites. Nature, 2018, 563, 541-545.	27.8	1,451
2	Thermodynamically stabilized Î²-CsPbI ₃ â€“based perovskite solar cells with efficiencies >18%. Science, 2019, 365, 591-595.	12.6	963
3	Highly Oriented Low-Dimensional Tin Halide Perovskites with Enhanced Stability and Photovoltaic Performance. Journal of the American Chemical Society, 2017, 139, 6693-6699.	13.7	723
4	Design of Lead-Free Inorganic Halide Perovskites for Solar Cells via Cation-Transmutation. Journal of the American Chemical Society, 2017, 139, 2630-2638.	13.7	714
5	Density functional study of FeS, FeSe, and FeTe: Electronic structure, magnetism, phonons, and superconductivity. Physical Review B, 2008, 78, .	3.2	690
6	Doping Lanthanide into Perovskite Nanocrystals: Highly Improved and Expanded Optical Properties. Nano Letters, 2017, 17, 8005-8011.	9.1	672
7	Strain engineering in perovskite solar cells and its impacts on carrier dynamics. Nature Communications, 2019, 10, 815.	12.8	528
8	Ultrasensitive detection of miRNA with an antimonene-based surface plasmon resonance sensor. Nature Communications, 2019, 10, 28.	12.8	475
9	Efficient and stable Ruddlesdenâ€“Popper perovskite solar cell with tailored interlayer molecular interaction. Nature Photonics, 2020, 14, 154-163.	31.4	443
10	Materials discovery at high pressures. Nature Reviews Materials, 2017, 2, .	48.7	427
11	Zn-Alloyed CsPbI₃ Nanocrystals for Highly Efficient Perovskite Light-Emitting Devices. Nano Letters, 2019, 19, 1552-1559.	9.1	395
12	Trifluoroacetate induced small-grained CsPbBr3 perovskite films result in efficient and stable light-emitting devices. Nature Communications, 2019, 10, 665.	12.8	350
13	Electronic correlations in the iron pnictides. Nature Physics, 2009, 5, 647-650.	16.7	317
14	Cuâ€“In Halide Perovskite Solar Absorbers. Journal of the American Chemical Society, 2017, 139, 6718-6725.	13.7	316
15	Atomically engineering activation sites onto metallic 1T-MoS2 catalysts for enhanced electrochemical hydrogen evolution. Nature Communications, 2019, 10, 982.	12.8	311
16	Rational Design of Halide Double Perovskites for Optoelectronic Applications. Joule, 2018, 2, 1662-1673.	24.0	297
17	Chlorine-Incorporation-Induced Formation of the Layered Phase for Antimony-Based Lead-Free Perovskite Solar Cells. Journal of the American Chemical Society, 2018, 140, 1019-1027.	13.7	241
18	Stabilizing Perovskite Solar Cells to IEC61215:2016 Standards with over 9,000-h Operational Tracking. Joule, 2020, 4, 2646-2660.	24.0	218

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19	Pressure-induced emission of cesium lead halide perovskite nanocrystals. Nature Communications, 2018, 9, 4506.	12.8	212
20	Colloidal Synthesis of Ternary Copper Halide Nanocrystals for High-Efficiency Deep-Blue Light-Emitting Diodes with a Half-Lifetime above 100 h. Nano Letters, 2020, 20, 3568-3576.	9.1	200
21	Stable Yellow Light-Emitting Devices Based on Ternary Copper Halides with Broadband Emissive Self-Trapped Excitons. ACS Nano, 2020, 14, 4475-4486.	14.6	199
22	Electrically-Driven Violet Light-Emitting Devices Based on Highly Stable Lead-Free Perovskite Cs₃Sb₂Br₉ Quantum Dots. ACS Energy Letters, 2020, 5, 385-394.	17.4	169
23	High Colorâ€Rendering Index and Stable White Lightâ€Emitting Diodes by Assembling Two Broadband Emissive Selfâ€Trapped Excitons. Advanced Materials, 2021, 33, e2001367.	21.0	162
24	Density functional study of excess Fe in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Fe</mml:mtext></mml:mrow><mml:mrow><mml:mn>1</mml:mn></mml:mr Magnetism and doping. Physical Review B, 2009, 79, .	3.2	156
25	Two-Dimensional PC₆ with Direct Band Gap and Anisotropic Carrier Mobility. Journal of the American Chemical Society, 2019, 141, 1599-1605.	13.7	144
26	Fast Diffusion of Native Defects and Impurities in Perovskite Solar Cell Material CH₃NH₃PbI₃. Chemistry of Materials, 2016, 28, 4349-4357.	6.7	139
27	CALYPSO structure prediction method and its wide application. Computational Materials Science, 2016, 112, 406-415.	3.0	138
28	Solid salt confinement effect: An effective strategy to fabricate high crystalline polymer carbon nitride for enhanced photocatalytic hydrogen evolution. Applied Catalysis B: Environmental, 2019, 246, 349-355.	20.2	136
29	Functionality-Directed Screening of Pb-Free Hybrid Organicâ€“Inorganic Perovskites with Desired Intrinsic Photovoltaic Functionalities. Chemistry of Materials, 2017, 29, 524-538.	6.7	135
30	Tellurium Hydrides at High Pressures: High-Temperature Superconductors. Physical Review Letters, 2016, 116, 057002.	7.8	132
31	Formation and Diffusion of Metal Impurities in Perovskite Solar Cell Material CH₃NH₃PbI₃: Implications on Solar Cell Degradation and Choice of Electrode. Advanced Science, 2018, 5, 1700662.	11.2	130
32	Thermochromic Leadâ€Free Halide Double Perovskites. Advanced Functional Materials, 2019, 29, 1807375.	14.9	120
33	Robust Stability of Efficient Lead-Free Formamidinium Tin Iodide Perovskite Solar Cells Realized by Structural Regulation. Journal of Physical Chemistry Letters, 2018, 9, 6999-7006.	4.6	117
34	CsPb(I Br1â^')3 solar cells. Science Bulletin, 2019, 64, 1532-1539.	9.0	114
35	Pseudohalideâ€Induced Recrystallization Engineering for CH₃NH₃PbI₃ Film and Its Application in Highly Efficient Inverted Planar Heterojunction Perovskite Solar Cells. Advanced Functional Materials, 2018, 28, 1704836.	14.9	112
36	Intrinsic Defect Properties in Halide Double Perovskites for Optoelectronic Applications. Physical Review Applied, 2018, 10, .	3.8	109

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37	Proton-transfer-induced 3D/2D hybrid perovskites suppress ion migration and reduce luminance overshoot. Nature Communications, 2020, 11, 3378.	12.8	108
38	Ba-induced phase segregation and band gap reduction in mixed-halide inorganic perovskite solar cells. Nature Communications, 2019, 10, 4686.	12.8	105
39	InSe: a two-dimensional material with strong interlayer coupling. Nanoscale, 2018, 10, 7991-7998.	5.6	102
40	Bulk heterojunction gifts bismuth-based lead-free perovskite solar cells with record efficiency. Nano Energy, 2020, 68, 104362.	16.0	102
41	A Unified Understanding of the Thickness-Dependent Bandgap Transition in Hexagonal Two-Dimensional Semiconductors. Journal of Physical Chemistry Letters, 2016, 7, 597-602.	4.6	100
42	First-principles study of electron-phonon coupling in hole- and electron-doped diamonds in the virtual crystal approximation. Physical Review B, 2005, 72, .	3.2	96
43	Perovskite Solar Absorbers: Materials by Design. Small Methods, 2018, 2, 1700316.	8.6	95
44	Materials discovery via CALYPSO methodology. Journal of Physics Condensed Matter, 2015, 27, 203203.	1.8	93
45	Bismuth and antimony-based oxyhalides and chalcohalides as potential optoelectronic materials. Npj Computational Materials, 2018, 4, .	8.7	86
46	Nanoporous Sulfur-Doped Copper Oxide (Cu₂O_xS_{1â€“x}) for Overall Water Splitting. ACS Applied Materials & Interfaces, 2018, 10, 745-752.	8.0	83
47	Wide InP Nanowires with Wurtzite/Zincblende Superlattice Segments Are Type-II whereas Narrower Nanowires Become Type-I: An Atomistic Pseudopotential Calculation. Nano Letters, 2010, 10, 4055-4060.	9.1	76
48	Evolution of Electronic Structure as a Function of Layer Thickness in Group-VIB Transition Metal Dichalcogenides: Emergence of Localization Prototypes. Nano Letters, 2015, 15, 949-957.	9.1	72
49	Stabilization of fullerene-like boron cages by transition metal encapsulation. Nanoscale, 2015, 7, 10482-10489.	5.6	72
50	Experimental Identification of Critical Condition for Drastically Enhancing Thermoelectric Power Factor of Two-Dimensional Layered Materials. Nano Letters, 2018, 18, 7538-7545.	9.1	72
51	Phase Diagram and High-Temperature Superconductivity of Compressed Selenium Hydrides. Scientific Reports, 2015, 5, 15433.	3.3	71
52	Computer-Assisted Inverse Design of Inorganic Electrides. Physical Review X, 2017, 7, .	8.9	70
53	Dielectric Behavior as a Screen in Rational Searches for Electronic Materials: Metal Pnictide Sulfosalts. Journal of the American Chemical Society, 2018, 140, 18058-18065.	13.7	69
54	High-Pressure Phase Stability and Superconductivity of Pnictogen Hydrides and Chemical Trends for Compressed Hydrides. Chemistry of Materials, 2016, 28, 1746-1755.	6.7	68

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55	Zintl-phase compounds with<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SnSb</mml:mtext></mml:mrow><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math> anions: Electronic structure and thermoelectric properties. Physical Review B, 2010, 81, .	3.2	66
56	Ab initio prediction of superconductivity in molecular metallic hydrogen under high pressure. Solid State Communications, 2007, 141, 610-614.	1.9	65
57	Ultrahigh-Performance Optoelectronics Demonstrated in Ultrathin Perovskite-Based Vertical Semiconductor Heterostructures. ACS Nano, 2019, 13, 7996-8003.	14.6	64
58	Ultrastable Leadâ€Free Double Perovskite Photodetectors with Imaging Capability. Advanced Materials Interfaces, 2019, 6, 1900188.	3.7	62
59	Bottom-up growth of homogeneous MoirÃ© superlattices in bismuth oxychloride spiral nanosheets. Nature Communications, 2019, 10, 4472.	12.8	59
60	Spontaneous low-temperature crystallization of Î±-FAPbI3 for highly efficient perovskite solar cells. Science Bulletin, 2019, 64, 1608-1616.	9.0	58
61	Electronic structure and thermoelectric properties of layered<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>PbSe-WSe</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> Physical Review B, 2009, 80, .	3.2	57
62	Electronic structure and thermoelectric properties:<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>PbBi</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> related intergrowth compounds. Physical Review B, 2010, 81, .	3.2	56
63	Genomic Design of Strong Direct-Gap Optical Transition in Si/Ge Core/Multishell Nanowires. Nano Letters, 2012, 12, 984-991.	9.1	54
64	Cdâ€Rich Alloyed CsPb<sub>1â€_xCd_xBr₃ Perovskite Nanorods with Tunable Blue Emission and Fermi Levels Fabricated through Crystal Phase Engineering. Advanced Science, 2020, 7, 2000930.	11.2	52
65	Highâ€throughput computational materials screening and discovery of optoelectronic semiconductors. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, .	14.6	52
66	Stacking Effects on Electronâ€“Phonon Coupling in Layered Hybrid Perovskites via Microstrain Manipulation. ACS Nano, 2020, 14, 5806-5817.	14.6	50
67	Genetic design of enhanced valley splitting towards a spin qubit in silicon. Nature Communications, 2013, 4, 2396.	12.8	49
68	N₂H: a novel polymeric hydronitrogen as a high energy density material. Journal of Materials Chemistry A, 2015, 3, 4188-4194.	10.3	49
69	Phonon instabilities in rocksalt AgCl and AgBr under pressure studied within density functional theory. Physical Review B, 2006, 74, .	3.2	45
70	Artificial control of in-plane anisotropic photoelectricity in monolayer MoS2. Applied Materials Today, 2019, 15, 203-211.	4.3	45
71	Discovery and ramifications of incidental MagnÃ©li phase generation and release from industrial coal-burning. Nature Communications, 2017, 8, 194.	12.8	44
72	Rod-shaped thiocyanate-induced abnormal band gap broadening in SCNâ¯ doped CsPbBr3 perovskite nanocrystals. Nano Research, 2018, 11, 2715-2723.	10.4	44

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73	Color Tunable Selfâ€Trapped Emissions from Leadâ€Free All Inorganic IAâ€IB Bimetallic Halides Csâ€Agâ€X (X = Cl,) Tj ETQq1 1 0.784	10.0	44
74	Electronic structure, localization, and spin-state transition in Cu-substituted<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>FeSe</mml:mtext><mml:mo>:</mml:mo><mml:msub><mml:mrow><mml:mtext>Fe</mml:m Physical Review B, 2010, 81, .	3.2	43
75	First-principles study of the lattice dynamics, thermodynamic properties and electron-phonon coupling of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Y</mml:mi><mml:msub><mml:mi mathvariant="normal">B</mml:mi><mml:mn>6</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2007, 76, .	3.2	42
76	Electronic structure ofBa(Fe,Ru)2As2andSr(Fe,Ir)2As2alloys. Physical Review B, 2009, 79, .	3.2	42
77	ATLAS: A real-space finite-difference implementation of orbital-free density functional theory. Computer Physics Communications, 2016, 200, 87-95.	7.5	42
78	Electronic structures, lattice dynamics, and electronâ€“phonon coupling of simple cubic Ca under pressure. Solid State Communications, 2008, 146, 181-185.	1.9	41
79	Phonon and elastic instabilities in rocksalt alkali hydrides under pressure: First-principles study. Physical Review B, 2007, 75, .	3.2	39
80	Density functional study of the overdoped iron chalcogenide<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TlFe</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:ms <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>ThCr</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:ms Physical Review B, 2009, 79, .	3.2	36
81	Intrinsic Transparent Conductors without Doping. Physical Review Letters, 2015, 115, 176602.	7.8	36
82	Alternative Loneâ€Pair ns²â€Cationâ€Based Semiconductors beyond Lead Halide Perovskites for Optoelectronic Applications. Advanced Materials, 2021, 33, e2008574.	21.0	34
83	CaCl2-type high-pressure phase of magnesium hydride predicted byab initiophonon calculations. Physical Review B, 2007, 75, .	3.2	33
84	New Polymorphs of 2D Indium Selenide with Enhanced Electronic Properties. Advanced Functional Materials, 2020, 30, 2001920.	14.9	33
85	Stable zero-dimensional cesium indium bromide hollow nanocrystals emitting blue light from self-trapped excitons. Nano Today, 2021, 38, 101153.	11.9	33
86	Computational functionalityâ€driven design of semiconductors for optoelectronic applications. InformaÄnÃ-MateriÃ¡ly, 2020, 2, 879-904.	17.3	32
87	Molecular engineering towards efficientwhite-light-emitting perovskite. Nature Communications, 2021, 12, 4890.	12.8	32
88	JAMIP: an artificial-intelligence aided data-driven infrastructure for computational materials informatics. Science Bulletin, 2021, 66, 1973-1985.	9.0	32
89	Halide Homogenization for High-Performance Blue Perovskite Electroluminescence. Research, 2020, 2020, 9017871.	5.7	32
90	Construction of crystal structure prototype database: methods and applications. Journal of Physics Condensed Matter, 2017, 29, 165901.	1.8	31

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91	Stable Cesium-Rich Formamidinium/Cesium Pure-Iodide Perovskites for Efficient Photovoltaics. ACS Energy Letters, 2021, 6, 2735-2741.	17.4	31
92	From Distortion to Disconnection: Linear Alkyl Diammonium Cations Tune Structure and Photoluminescence of Lead Bromide Perovskites. Advanced Optical Materials, 2020, 8, 1902051.	7.3	30
93	Extraordinary Temperature Dependent Second Harmonic Generation in Atomically Thin Layers of Transitionâ€Metal Dichalcogenides. Advanced Optical Materials, 2020, 8, 2000441.	7.3	30
94	Tuning optical properties of transparent conducting barium stannate by dimensional reduction. APL Materials, 2015, 3, .	5.1	29
95	Design of ternary alkaline-earth metal Sn(<scp>ii</scp>) oxides with potential good p-type conductivity. Journal of Materials Chemistry C, 2016, 4, 4592-4599.	5.5	29
96	Anatase (101)-like Structural Model Revealed for Metastable Rutile TiO₂(011) Surface. ACS Applied Materials & Interfaces, 2017, 9, 7891-7896.	8.0	29
97	Interlayer coupling in two-dimensional semiconductor materials. Semiconductor Science and Technology, 2018, 33, 093001.	2.0	29
98	Dimension Engineering of High-Quality InAs Nanostructures on a Wafer Scale. Nano Letters, 2019, 19, 1632-1642.	9.1	29
99	Halogen Substitution in Zeroâ€Đimensional Mixed Metal Halides toward Photoluminescence Modulation and Enhanced Quantum Yield. Advanced Optical Materials, 2020, 8, 2000418.	7.3	29
100	Band structure engineering through van der Waals heterostructing superlattices of <scp>twoâ€dimensional</scp> transition metal dichalcogenides. InformaÄnÃ-MateriÃ¡ly, 2021, 3, 201-211.	17.3	27
101	Imaging of the Atomic Structure of All-Inorganic Halide Perovskites. Journal of Physical Chemistry Letters, 2020, 11, 818-823.	4.6	26
102	Pressure-induced enhancement of electron-phonon coupling in superconductingCaC6from first principles. Physical Review B, 2006, 74, .	3.2	25
103	Observation of excitonic series in monolayer and few-layer black phosphorus. Physical Review B, 2020, 101, .	3.2	25
104	High-pressure phase transformations in CaH2. Journal of Physics Condensed Matter, 2008, 20, 045211.	1.8	24
105	Density functional study of the electronic structure and magnetism of LaFeAsO alloyed with Zn. Physical Review B, 2009, 80, .	3.2	24
106	Absence of intrinsic spin splitting in one-dimensional quantum wires of tetrahedral semiconductors. Physical Review B, 2011, 84, .	3.2	24
107	First-principles study of the pressure-induced rutileâ€“CaCl2 phase transition in MgF2. Solid State Communications, 2008, 145, 283-287.	1.9	23
108	Effects of manganese doping on the structure evolution of small-sized boron clusters. Journal of Physics Condensed Matter, 2017, 29, 265401.	1.8	23

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109	Intrinsic ultralow lattice thermal conductivity of the unfilled skutterudite<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>FeSb</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2016, 94, .	3.2	22
110	Design of Mixedâ€Cation Triâ€Layered Pbâ€Free Halide Perovskites for Optoelectronic Applications. Advanced Electronic Materials, 2019, 5, 1900234.	5.1	21
111	The Introduction of Defects in Ti₃C₂T_x and Ti₃C₂T_xâ€Assisted Reduction of Graphene Oxide for Highly Selective Detection of ppbâ€Level NO₂. Advanced Functional Materials, 2022, 32, .	14.9	21
112	Switchable Outâ€ofâ€Plane Polarization in 2D LiAlTe₂. Advanced Electronic Materials, 2019, 5, 1900089.	5.1	20
113	Impact of organic molecule rotation on the optoelectronic properties of hybrid halide perovskites. Physical Review Materials, 2019, 3, .	2.4	20
114	Metal Halide Semiconductors beyond Lead-Based Perovskites for Promising Optoelectronic Applications. Journal of Physical Chemistry Letters, 2021, 12, 10532-10550.	4.6	20
115	Stability, electronic structures and thermoelectric properties of binary Znâ€“Sb materials. Journal of Materials Chemistry C, 2016, 4, 11305-11312.	5.5	19
116	First-principle high-throughput calculations of carrier effective masses of two-dimensional transition metal dichalcogenides. Journal of Semiconductors, 2018, 39, 072001.	3.7	18
117	Van der Waals SnSe 2(1â^' x) S 2 x Alloys: Compositionâ€Dependent Bowing Coefficient and Electronâ€“Phonon Interaction. Advanced Functional Materials, 2020, 30, 1908092.	14.9	18
118	Stable and luminescent halide perovskite fabricated in water. Light: Science and Applications, 2020, 9, 106.	16.6	18
119	Pressureâ€Tailored Band Engineering for Significant Enhancements in the Photoelectric Performance of CsI₃ in the Optical Communication Waveband. Advanced Functional Materials, 2022, 32, 2108636.	14.9	18
120	Possible superconductivity in Fe-Sb based materials: Density functional study of LiFeSb. Physical Review B, 2008, 78, .	3.2	17
121	Sn(II)-Containing Phosphates as Optoelectronic Materials. Chemistry of Materials, 2017, 29, 2459-2465.	6.7	17
122	Discovery of New Polymorphs of Gallium Oxides with Particle Swarm Optimizationâ€Based Structure Searches. Advanced Electronic Materials, 2020, 6, 2000119.	5.1	17
123	Enhanced Optical Emission from 2D InSe Bent onto Siâ€Pillars. Advanced Optical Materials, 2020, 8, 2000828.	7.3	17
124	Excitons and excitonic fine structures in Si nanowires: Prediction of an electronic state crossover with diameter changes. Physical Review B, 2011, 84, .	3.2	15
125	The Birth of a Type-II Nanostructure: Carrier Localization and Optical Properties of Isoelectronically Doped CdSe:Te Nanocrystals. ACS Nano, 2012, 6, 8325-8334.	14.6	15
126	Rational design of new phases of tin monosulfide by first-principles structure searches. Science China: Physics, Mechanics and Astronomy, 2018, 61, 1.	5.1	15

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127	Thermal Shock Fabrication of Ionâ€Stabilized Perovskite and Solar Cells. Advanced Materials, 2022, 34, .	21.0	15
128	<scp>Pb₅Sb₈S₁₇</scp> quantum dotâ€sensitized solar cells with an efficiency of 6% under 0.05 sun: <scp>T</scp>heoretical and experimental studies. Progress in Photovoltaics: Research and Applications, 2018, 26, 205-213.	8.1	13
129	Global instability index as a crystallographic stability descriptor of halide and chalcogenide perovskites. Journal of Energy Chemistry, 2022, 70, 1-8.	12.9	13
130	First-principles investigation of structural and electronic properties of oxygen adsorbing phosphorene. Progress in Natural Science: Materials International, 2019, 29, 316-321.	4.4	12
131	Collective-Goldstone-mode-induced ultralow lattice thermal conductivity in Sn-filled skutterudite <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>SnFe</mml:mi><mml:mn>4</mml:mn></ Physical Review B, 2018, 97, .	3.2	11
132	Computational Design of Mixed-Valence Tin Sulfides as Solar Absorbers. ACS Applied Materials & Interfaces, 2019, 11, 24867-24875.	8.0	11
133	Rashba band splitting in two-dimensional Ruddlesdenâ€“Popper halide perovskites. Journal of Applied Physics, 2020, 128, 175101.	2.5	11
134	Diverse electronic properties of 2D layered Se-containing materials composed of quasi-1D atomic chains. Physical Chemistry Chemical Physics, 2020, 22, 2122-2129.	2.8	10
135	New stable ternary alkaline-earth metal Pb(II) oxides: <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mrow><mml:mi>Ca</mml:mi><mml:mo>/</m mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BaPbO</mml:mi><mml:mn>2</mml:mn></mml:msub> Physical Review Materials, 2017, 1, .	2.4	10
136	Reinterpretation of the Expected Electronic Density of States of Semiconductor Nanowires. Nano Letters, 2015, 15, 88-95.	9.1	9
137	Sn2Se3: A conducting crystalline mixed valent phase change memory compound. Journal of Applied Physics, 2017, 121, .	2.5	9
138	Grain Boundaries in Methylammonium Lead Halide Perovskites Facilitate Water Diffusion. Advanced Energy and Sustainability Research, 2021, 2, 2100087.	5.8	9
139	Structural, Thermodynamical and Electronic Properties of All-Inorganic Lead Halide Perovskites. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2020, .	4.9	9
140	Evaluation of performance of machine learning methods in mining structureâ€“property data of halide perovskite materials. Chinese Physics B, 2022, 31, 056302.	1.4	8
141	High-throughput computational material screening of the cycloalkane-based two-dimensional Dionâ€“Jacobson halide perovskites for optoelectronics. Chinese Physics B, 2022, 31, 037104.	1.4	8
142	Optical emission enhancement of bent InSe thin films. Science China Information Sciences, 2021, 64, 1.	4.3	6
143	Phase transition pathway of hybrid halide perovskites under compression: Insights from first-principles calculations. Physical Review Materials, 2021, 5, .	2.4	6
144	Helium incorporation induced direct-gap silicides. Npj Computational Materials, 2021, 7, .	8.7	6

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145	Proton Transferâ€Driven Modification of 3D Hybrid Perovskites to Form Oriented 2D Ruddlesdenâ€“Popper Phases. Small Science, 2022, 2, .	9.9	6
146	Perovskite Photovoltaics: Pseudohalideâ€Induced Recrystallization Engineering for CH₃NH₃PbI₃ Film and Its Application in Highly Efficient Inverted Planar Heterojunction Perovskite Solar Cells (Adv. Funct. Mater. 2/2018). Advanced Functional Materials, 2018, 28, 1870013.	14.9	5
147	White Lightâ€Emitting Diodes: High Colorâ€Rendering Index and Stable White Lightâ€Emitting Diodes by Assembling Two Broadband Emissive Selfâ€Trapped Excitons (Adv. Mater. 2/2021). Advanced Materials, 2021, 33, 2170010.	21.0	5
148	Dopability of divalent tin containing phosphates for <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>p</mml:mi></mml:math> -type transparent conductors. Physical Review Materials, 2019, 3, .	2.4	5
149	Two-dimensional Ruddlesden-Popper halide perovskite solar absorbers with short-chain interlayer spacers. Physical Review Materials, 2022, 6, .	2.4	5
150	Preface to the Special Issue on 2D-Materials-Related Physical Properties and Optoelectronic Devices. Journal of Semiconductors, 2019, 40, 060101.	3.7	4
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152	Entropy-Driven Stabilization of Multielement Halide Double-Perovskite Alloys. Journal of Physical Chemistry Letters, 0, , 5017-5024.	4.6	4
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