Shiyou Chen

List of Publications by Year
in descending order

164 papers	15,496 citations	19608 61 h-index	17546 121 g-index
169 all docs	169 docs citations	169 times ranked	13000 citing authors

#	Article	IF	Citations
1	Classification of Lattice Defects in the Kesterite Cu₂ZnSnS₄ and Cu₂ZnSnSe₄ Earthâ€Abundant Solar Cell Absorbers. Advanced Materials, 2013, 25, 1522-1539.	11.1	1,210
2	Thin-film Sb2Se3 photovoltaics with oriented one-dimensional ribbons and benign grain boundaries. Nature Photonics, 2015, 9, 409-415.	15.6	781
3	Thermodynamic Oxidation and Reduction Potentials of Photocatalytic Semiconductors in Aqueous Solution. Chemistry of Materials, 2012, 24, 3659-3666.	3.2	627
4	Intrinsic point defects and complexes in the quaternary kesterite semiconductor<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Cu</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msu Physical Review B, 2010, 81, .	1.1	624
5	Cu2ZnSnS4 solar cells with over 10% power conversion efficiency enabled by heterojunction heat treatment. Nature Energy, 2018, 3, 764-772.	19.8	623
6	Kesterite Thinâ€Film Solar Cells: Advances in Materials Modelling of Cu₂ZnSnS₄. Advanced Energy Materials, 2012, 2, 400-409.	10.2	589
7	Crystal and electronic band structure of Cu2ZnSnX4 (X=S and Se) photovoltaic absorbers: First-principles insights. Applied Physics Letters, 2009, 94, .	1.5	585
8	Selfâ€Regulation Mechanism for Charged Point Defects in Hybrid Halide Perovskites. Angewandte Chemie - International Edition, 2015, 54, 1791-1794.	7.2	484
9	Defect physics of the kesterite thin-film solar cell absorber Cu2ZnSnS4. Applied Physics Letters, 2010, 96, .	1.5	454
10	Electronic structure and stability of quaternary chalcogenide semiconductors derived from cation cross-substitution of II-VI and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>I-III-VI</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:m Physical Review B, 2009, 79, .	1.1	413
11	Hybrid functional study of structural and electronic properties of Cu<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>ZnSn(S,Se)<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>4</mml:mn></mml:mrow>	1.1	399
12	Hydrothermal deposition of antimony selenosulfide thin films enables solar cells with 10% efficiency. Nature Energy, 2020, 5, 587-595.	19.8	338
13	Engineering Solar Cell Absorbers by Exploring the Band Alignment and Defect Disparity: The Case of Cuâ€• and Agâ€Based Kesterite Compounds. Advanced Functional Materials, 2015, 25, 6733-6743.	7.8	284
14	CuSbS₂ as a Promising Earth-Abundant Photovoltaic Absorber Material: A Combined Theoretical and Experimental Study. Chemistry of Materials, 2014, 26, 3135-3143.	3.2	278
15	Wurtzite-derived polytypes of kesterite and stannite quaternary chalcogenide semiconductors. Physical Review B, 2010, 82, .	1.1	259
16	Influence of Defects and Synthesis Conditions on the Photovoltaic Performance of Perovskite Semiconductor CsSnI₃. Chemistry of Materials, 2014, 26, 6068-6072.	3.2	256
17	GeSe Thin-Film Solar Cells Fabricated by Self-Regulated Rapid Thermal Sublimation. Journal of the American Chemical Society, 2017, 139, 958-965.	6.6	238
18	Furfuraldehyde Hydrogenation on Titanium Oxide-Supported Platinum Nanoparticles Studied by Sum Frequency Generation Vibrational Spectroscopy: Acidâ€“Base Catalysis Explains the Molecular Origin of Strong Metalâ€“Support Interactions. Journal of the American Chemical Society, 2012, 134, 14208-14216.	6.6	198

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19	Facile Preparation of Light Emitting Organic Metal Halide Crystals with Near-Unity Quantum Efficiency. Chemistry of Materials, 2018, 30, 2374-2378.	3.2	193
20	Revised ab initio natural band offsets of all group IV, II-VI, and III-V semiconductors. Applied Physics Letters, 2009, 94, .	1.5	188
21	Effective band gap narrowing of anatase TiO2 by strain along a soft crystal direction. Applied Physics Letters, 2010, 96, .	1.5	185
22	Composition dependence of structure and optical properties of Cu2ZnSn(S,Se)4 solid solutions: An experimental study. Journal of Alloys and Compounds, 2012, 511, 129-132.	2.8	181
23	Abundance of CuZnâ€‰+â€‰SnZn and 2CuZnâ€‰+â€‰SnZn defect clusters in kesterite solar cells. Applied Physics Letters, 2012, 101, .	1.5	178
24	Unraveling luminescence mechanisms in zero-dimensional halide perovskites. Journal of Materials Chemistry C, 2018, 6, 6398-6405.	2.7	168
25	Structural, optical, and electronic properties of Cu<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>Sn<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"		

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37	CuSbSe₂ as a Potential Photovoltaic Absorber Material: Studies from Theory to Experiment. Advanced Energy Materials, 2015, 5, 1501203.	10.2	99
38	Influence of defects and dopants on the photovoltaic performance of Bi₂S₃: first-principles insights. Journal of Materials Chemistry A, 2017, 5, 6200-6210.	5.2	97
39	Organicâ"Inorganic Layered and Hollow Tin Bromide Perovskite with Tunable Broadband Emission. ACS Applied Materials & Interfaces, 2018, 10, 34363-34369.	4.0	97
40	Deciphering Halogen Competition in Organometallic Halide Perovskite Growth. Journal of the American Chemical Society, 2016, 138, 5028-5035.	6.6	92
41	Cu<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>Zn(Sn,Ge)Se<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>and Cu<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow	1.1	90
42	Composition- and Band-Gap-Tunable Synthesis of Wurtzite-Derived Cu₂ZnSn(S_{1â€"x}Se_x)₄ Nanocrystals: Theoretical and Experimental Insights. ACS Nano, 2013, 7, 1454-1463.	7.3	89
43	Phase Stability and Defect Physics of a Ternary ZnSnN₂ Semiconductor: First Principles Insights. Advanced Materials, 2014, 26, 311-315.	11.1	81
44	Emerging Chalcogenide Thin Films for Solar Energy Harvesting Devices. Chemical Reviews, 2022, 122, 10170-10265.	23.0	81
45	Intrinsic Defect Limit to the Electrical Conductivity and a Twoâ€Step pâ€Type Doping Strategy for Overcoming the Efficiency Bottleneck of Sb₂S₃â€Based Solar Cells. Solar Rrl, 2020, 4, 1900503.	3.1	79
46	Defect Engineering in Earthâ€Abundant Cu₂ZnSn(S,Se)₄ Photovoltaic Materials via Ga³⁺â€Doping for over 12% Efficient Solar Cells. Advanced Functional Materials, 2021, 31, 2010325.	7.8	79
47	Bandgap Tunability in Zn(Sn,Ge)N₂ Semiconductor Alloys. Advanced Materials, 2014, 26, 1235-1241.	11.1	75
48	First-principles study on the effective masses of zinc-blend-derived Cu2Znâ"IVâ"VI4 (IVâ€‰=â€‰Sn, Ge, Si) Tj ETQq0 0 0 rgBT /	1.1	74
49	Copperâ€alloyed ZnS as a pâ€type transparent conducting material. Physica Status Solidi (A) Applications and Materials Science, 2012, 209, 2101-2107.	0.8	73
50	Effective and Noneffective Recombination Center Defects in Cu₂ZnSnS₄: Significant Difference in Carrier Capture Cross Sections. Chemistry of Materials, 2019, 31, 826-833.	3.2	72
51	Superhard PseudocubicBC2NSuperlattices. Physical Review Letters, 2007, 98, 015502.	2.9	71
52	Broadband Emission in Hybrid Organicâ€"Inorganic Halides of Group 12 Metals. ACS Omega, 2018, 3, 18791-18802.	1.6	70
53	Origin of Reduced Efficiency in Cu(In,Ga)Se$_2$ Solar Cells With High Ga Concentration: Alloy Solubility Versus Intrinsic Defects. IEEE Journal of Photovoltaics, 2014, 4, 477-482.	1.5	69
54	Single-step preparation and characterization of Cu2ZnSn(SxSe1â"x)4 thin films deposited by pulsed laser deposition method. Journal of Alloys and Compounds, 2012, 529, 34-37.	2.8	68

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55	The Role of Hydrogen from ALDâ€Al₂O₃ in Kesterite Cu₂ZnSnS₄ Solar Cells: Grain Surface Passivation. Advanced Energy Materials, 2018, 8, 1701940.	10.2	68
56	Inâ€Plane Optical Anisotropy of Lowâ€Symmetry 2D GeSe. Advanced Optical Materials, 2019, 7, 1801311.	3.6	68
57	Chemical Trends in the Thermodynamic Stability and Band Gaps of 980 Halide Double Perovskites: A High-Throughput First-Principles Study. ACS Applied Materials & Interfaces, 2020, 12, 20680-20690.	4.0	68
58	Pt-Mediated Reversible Reduction and Expansion of CeO₂ in Pt Nanoparticle/Mesoporous CeO₂ Catalyst: In Situ X-ray Spectroscopy and Diffraction Studies under Redox (H₂ and O₂) Atmospheres. Journal of Physical Chemistry C, 2013, 117, 26608-26616.	1.5	67
59	Chemical instability leads to unusual chemical-potential-independent defect formation and diffusion in perovskite solar cell material CH₃NH₃PbI₃. Journal of Materials Chemistry A, 2016, 4, 16975-16981.	5.2	67
60	Zero-dimensional Cs₄EuX₆ (X = Br, I) all-inorganic perovskite single crystals for gamma-ray spectroscopy. Journal of Materials Chemistry C, 2018, 6, 6647-6655.	2.7	66
61	Bulk Assembly of Corrugated 1D Metal Halides with Broadband Yellow Emission. Advanced Optical Materials, 2019, 7, 1801474.	3.6	65
62	Origin of Band-Tail and Deep-Donor States in Cu₂ZnSnS₄ Solar Cells and Their Suppression through Sn-Poor Composition. Journal of Physical Chemistry Letters, 2019, 10, 7929-7936.	2.1	64
63	Band structure engineering of multinary chalcogenide topological insulators. Physical Review B, 2011, 83, .	1.1	60
64	Impact of metal <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">n</mml:mi><mml:msup><mml:mrow><mml:mi mathvariant="normal">s</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msup></mml:mrow></mml:math> lone pair on luminescence quantum efficiency in low-dimensional halide perovskites. Physical Review Materials, 2019, 3, .	0.9	60
65	Antiferromagnetic ground state with pair-checkerboard order in FeSe. Physical Review B, 2015, 91, .	1.1	59
66	An antibonding valence band maximum enables defect-tolerant and stable GeSe photovoltaics. Nature Communications, 2021, 12, 670.	5.8	58
67	High Efficiency Cu₂ZnSn(S,Se)₄ Solar Cells with Shallow Li_{Zn} Acceptor Defects Enabled by Solutionâ€Based Li Postâ€Deposition Treatment. Advanced Energy Materials, 2021, 11, 2003783.	10.2	57
68	Sodium Passivation of the Grain Boundaries in CuInSe₂ and Cu₂ZnSnS₄ for Highâ€Efficiency Solar Cells. Advanced Energy Materials, 2017, 7, 1601457.	10.2	56
69	Electronic structure and phase stability of MgTe, ZnTe, CdTe, and their alloys in theB3,B4, andB8 structures. Physical Review B, 2009, 79, .	1.1	55
70	Stability and electronic structure of Cu<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>ZnSnS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>surfaces: First-principles study. Physical Review B, 2013, 88, .	1.1	55
71	Inverse design of materials by multi-objective differential evolution. Computational Materials Science, 2015, 98, 51-55.	1.4	55
72	Polytypic Nanocrystals of Cu-Based Ternary Chalcogenides: Colloidal Synthesis and Photoelectrochemical Properties. Journal of the American Chemical Society, 2016, 138, 5576-5584.	6.6	54

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73	Solution-based synthesis and characterization of Cu2FeSnS4 nanocrystals. Materials Chemistry and Physics, 2012, 133, 688-691.	2.0	48
74	Linearly arranged polytypic CZTSSe nanocrystals. Scientific Reports, 2012, 2, 952.	1.6	45
75	Predicting the thermodynamic stability of double-perovskite halides from density functional theory. APL Materials, 2018, 6, .	2.2	42
76	Indolo[3,2,1-jk]carbazole Derivatives-Sensitized Solar Cells: Effect of Ï€-Bridges on the Performance of Cells. Journal of Physical Chemistry C, 2014, 118, 14211-14217.	1.5	41
77	Cu-deficiency induced structural transition of Cu_{2â^'x}Te. CrystEngComm, 2015, 17, 2878-2885.	1.3	41
78	Oxygen Vacancy Induced Flat Phonon Mode at FeSe /SrTiO3 interface. Scientific Reports, 2015, 5, 10011.	1.6	39
79	Intrinsic Defect Limit to the Growth of Orthorhombic HfO₂ and (Hf,Zr)O₂ with Strong Ferroelectricity: Firstâ€Principles Insights. Advanced Functional Materials, 2021, 31, 2104913.	7.8	39
80	Temperature dependence of phonon modes, dielectric functions, and interband electronic transitions in Cu2ZnSnS4 semiconductor films. Physical Chemistry Chemical Physics, 2012, 14, 9936.	1.3	38
81	Crystal structures and mechanical properties of superhard <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">B</mml:mi><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">N</mml:mi></mml:mrow></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant	1.1	35
82	Rb₄Ag₂BiBr₉: A Lead-Free Visible Light Absorbing Halide Semiconductor with Improved Stability. Inorganic Chemistry, 2019, 58, 4446-4455.	1.9	35
83	Intrinsic defects and electronic conductivity of TaON: First-principles insights. Applied Physics Letters, 2011, 99, .	1.5	34
84	Si:WO3heterostructure for Z-scheme water splitting: an ab initio study. Journal of Materials Chemistry A, 2013, 1, 1078-1085.	5.2	32
85	Three-step approach for computing band offsets and its application to inorganic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mrow><mml:mi>A</mml:mi><mml:mi>B</mml:mi></mml:mrow></mml:mr perovskites. Physical Review B, 2015, 92, .	3.1	32
86	Quasi-one-dimensional Sb2(S,Se)3 alloys as bandgap-tunable and defect-tolerant photocatalytic semiconductors. Journal of Chemical Physics, 2020, 153, 014703.	1.2	32
87	More Se Vacancies in Sb₂Se₃ under Seâ€Rich Conditions: An Abnormal Behavior Induced by Defectâ€Correlation in Compensated Compound Semiconductors. Small, 2021, 17, e2102429.	5.2	32
88	Hybrid crystalline sp 2 sp 3 carbon as a high-efficiency solar cell absorber. Carbon, 2016, 109, 246-252.	5.4	31
89	Halide Doubleâ€Perovskite Lightâ€Emitting Centers Embedded in Latticeâ€Matched and Coherent Crystalline Matrix. Advanced Functional Materials, 2020, 30, 2000653.	7.8	30
90	Double-hole-induced oxygen dimerization in transition metal oxides. Physical Review B, 2014, 89, .	1.1	26

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91	Indirect-direct band gap transition of two-dimensional arsenic layered semiconductorsâ€"cousins of black phosphorus. Science China: Physics, Mechanics and Astronomy, 2015, 58, 1.	2.0	26
92	DASP: Defect and Dopant ab-initio Simulation Package. Journal of Semiconductors, 2022, 43, 042101.	2.0	25
93	Organicâ€"inorganic hybrid perovskite scintillators for mixed field radiation detection. InformaÄnÃ-MateriÃ¡ly, 2022, 4, .	8.5	25
94	First-principles study of defect properties of zinc blende MgTe. Physical Review B, 2011, 83, .	1.1	24
95	High-stability fluorescent perovskites embedded in PbBrOH triggered by imidazole derivatives in water. Journal of Materials Chemistry C, 2020, 8, 5594-5599.	2.7	24
96	Cation-Mutation Design of Quaternary Nitride Semiconductors Lattice-Matched to GaN. Chemistry of Materials, 2015, 27, 7757-7764.	3.2	23
97	Hydrazine solution processed CuSbSe2: Temperature dependent phase and crystal orientation evolution. Solar Energy Materials and Solar Cells, 2017, 168, 112-118.	3.0	23
98	Crystal structure and defect reactions in the kesterite solar cell absorber Cu[sub 2]ZnSnS[sub 4] (CZTS): Theoretical insights. , 2011, , .		22
99	Self-passivation rule and structure of CdTe Î£3 (112) grain boundaries. Physical Review B, 2016, 93, .	1.1	21
100	Calculation studies on point defects in perovskite solar cells. Journal of Semiconductors, 2017, 38, 011006.	2.0	20
101	Boosting the Electrochemical Performance of Allâ€Solidâ€State Batteries with Sulfide Li₆PS₅Cl Solid Electrolyte Using Li₂WO₄â€Coated LiCoO₂ Cathode. Advanced Materials Interfaces, 2021, 8, 2100624.	1.9	20
102	Evolution of anatase surface active sites probed by in situ sum-frequency phonon spectroscopy. Science Advances, 2016, 2, e1601162.	4.7	19
103	Interfacial engineering to improve Cu2ZnSnX4 (X = S, Se) solar cell efficiency. APL Materials, 2019, 7, .	2.2	19
104	Dissociation path competition of radiolysis ionization-induced molecule damage under electron beam illumination. Chemical Science, 2019, 10, 10706-10715.	3.7	19
105	Lead-free hybrid perovskite N(CH3)4SnI3 with robust ferroelectricity induced by large and non-polar N(CH3)4+ molecular cation. Nature Communications, 2021, 12, 637.	5.8	19
106	Extrinsic dopants in quasi-one-dimensional photovoltaic semiconductor Sb2S3: A first-principles study. Journal of Applied Physics, 2020, 127, 183101.	1.1	19
107	Comprehensive investigations on charge diffusion physics in SiN-based 3D NAND flash memory through systematical Ab initio calculations. , 2017, , .		18
108	Prediction of (TiO₂)_x(Cu₂O)_yalloys for efficient photoelectrochemical water splitting. Physical Chemistry Chemical Physics, 2013, 15, 1778-1781.	1.3	17

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109	First-principles study on the alkali chalcogenide secondary compounds in Cu(In,Ga)Se2 and Cu2ZnSn(S,Se)4 thin film solar cells. Journal of Energy Chemistry, 2018, 27, 1140-1150.	7.1	16
110	Chemical Trend of Transition-Metal Doping in WSe2. Physical Review Applied, 2019, 12, .	1.5	16
111	Natural Intermediate Band in I 2 -II-IV-VI4 Quaternary Chalcogenide Semiconductors. Scientific Reports, 2018, 8, 1604.	1.6	15
112	Temperature Dependence of Phonon Modes, Optical Constants, and Optical Band Gap in Two-Dimensional ReS2 Films. Journal of Physical Chemistry C, 2018, 122, 29464-29469.	1.5	15
113	Defect Physics of Ternary Semiconductor <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mrow><mml:mi>Zn</mml:mi><mml:mi>Ge</mml:mi><mml:mi mathvariant="normal">P</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:math> with a High Density of Anion-Cation Antisites: A First-Principles Study. Physical Review Applied, 2021, 15, .	1.5	15
114	Quaternary semiconductors with positive crystal field splitting: Potential high-efficiency spin-polarized electron sources. Applied Physics Letters, 2009, 95, .	1.5	14
115	First-principles exploration of defect-pairs in GaN. Journal of Semiconductors, 2020, 41, 032104.	2.0	14
116	Giant biquadratic interaction-induced magnetic anisotropy in the iron-based superconductor<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>A</mml:mi><mml:mi>x</mml:mi></mml:msub><mml:msub><mml:mi mathvariant="normal">F</mml:mi><mml:msub><mml:mi mathvariant="normal">e</mml:mi><mml:mrow><mml:mn>2</mml:mn><mml:mo>â^’</mml:mo><mml:mi>y</mml:mi></mml:mrow></mml:msub><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mi mathvariant="normal">e</mml:mi></mml:msub></mml:mrow></mml:math>	1.1	13
117	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">P</mml:mi><mml:msub><mml:mi mathvariant="normal">b</mml:mi><mml:mi mathvariant="normal">I</mml:mi></mml:msub></mml:mrow></mml:math> antisite in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi mathvariant="normal">C</mml:mi><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mi mathvariant="normal">N</mml:mi><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mi mathvariant="normal">P</mml:mi><mml:msub><mml:mi mathvariant="normal">I</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>	1.1	13
118	Hierarchically Structured Thermoelectric Materials in Quaternary System Cuâ€“Znâ€“Snâ€“S Featuring a Mosaic-type Nanostructure. ACS Applied Nano Materials, 2018, 1, 2579-2588.	2.4	13
119	High-throughput first-principles screening of layered magnetic double perovskites Cs₄MSb₂X₁₂ for spintronic applications. Journal of Physics Condensed Matter, 2020, 32, 225705.	0.7	12
120	pâ€Type Antimony Selenide via Lead Doping. Solar Rrl, 2022, 6, 2100730.	3.1	12
121	Evolution of the Interfacial Layer and Its Impact on Electric-Field-Cycling Behaviors in Ferroelectric Hf_{1â€“x}Zr_xO₂. ACS Applied Materials & Interfaces, 2022, 14, 11028-11037.	4.0	12
122	Origin of the type-II band offset between rutile and anatase titanium dioxide: Classical and quantum-mechanical interactions between O ions. Physical Review B, 2017, 95, .	1.1	11
123	High-throughput screening and classification of layered di-metal chalcogenides. Nanoscale, 2019, 11, 13924-13933.	2.8	11
124	NaSbSe2 as a promising light-absorber semiconductor in solar cells: First-principles insights. APL Materials, 2019, 7, 081122.	2.2	11
125	Absolute Volume Deformation Potentials of Inorganic ABX₃ Halide Perovskites: The Chemical Trends. Advanced Theory and Simulations, 2021, 4, 2100060.	1.3	11
126	Ground-state structure of coherent lattice-mismatched zinc-blendeA1â^’xBxCsemiconductor alloys (x=0.25and 0.75). Physical Review B, 2008, 77, .	1.1	10

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127	Optoelectronic properties of candidate photovoltaic Cu2PbSiS4, Ag2PbGeS4 and KAg2SbS4 semiconductors. Journal of Alloys and Compounds, 2018, 746, 405-412.	2.8	10
128	Theoretical study on the kesterite solar cells based on Cu ₂ ZnSn(S,Se) ₄ and related photovoltaic semiconductors. Chinese Physics B, 2018, 27, 018806.	0.7	10
129	Low Electron Carrier Concentration Near the pâ€n Junction Interface: A Fundamental Factor Limiting Shortâ€Circuit Current of Cu(In,Ga)Se₂ Solar Cells. Solar Rrl, 2019, 3, 1900057.	3.1	10
130	Design of Multifunctional Quinternary Metal-Halide Perovskite Compounds Based on Cationâ€“Anion Co-Ordering. Chemistry of Materials, 2020, 32, 5949-5957.	3.2	10
131	Energy-dependent knock-on damage of organicâ€“inorganic hybrid perovskites under electron beam irradiation: First-principles insights. Applied Physics Letters, 2021, 119, .	1.5	10
132	Chen, Gong, and Wei Reply:. Physical Review Letters, 2007, 99, .	2.9	9
133	Polaron-enhanced giant strain effect on defect formation: The case of oxygen vacancies in rutile <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>TiO</mml:mi><mml:mn>2</mml:mn></mml:msub></m Physical Review B, 2019, 99, .	1.1	8
134	Earth-abundant photovoltaic semiconductor NaSbS2 in the rocksalt-derived structure: A first-principles study. Progress in Natural Science: Materials International, 2019, 29, 322-328.	1.8	8
135	Role of Lithium Codoping in Enhancing the Scintillation Yield of Aluminate Garnets. Physical Review Applied, 2020, 13, .	1.5	8
136	Defect-assisted nonradiative recombination in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Cu</mml:mi><mml:mn>2</mml:mn></mml: : A comparative study with <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Cu</mml:mi><mml:mn>2</mml:mn></mml: mathvariant="normal">S</mml:mi><mml:mn>4</mml:. Physical Review Materials, 2021, 5, .	0.9	8
137	Role of Polycyclic Aromatic Alkylammonium Cations in Tuning the Electronic Properties and Band Alignment of Two-Dimensional Hybrid Perovskite Semiconductors. Journal of Physical Chemistry Letters, 2021, 12, 9754-9760.	2.1	8
138	Design of quaternary chalcogenide photovoltaic absorbers through cation mutation. , 2009, , .		7
139	First-principles identification of V_IÂ+ÂCu_i defect cluster in cuprous iodide: origin of red light photoluminescence. Nanotechnology, 2022, 33, 195203.	1.3	7
140	Anisotropic in-plane thermal conductivity in multilayer silicene. Physics Letters, Section A: General, Atomic and Solid State Physics, 2018, 382, 1499-1503.	0.9	6
141	Configuration dependence of the electronic structure and optical properties of BC₂N alloys. Physica Status Solidi (B): Basic Research, 2009, 246, 589-593.	0.7	5
142	Structural, Electronic and Defect Properties of Cu2ZnSn(S,Se)4 Alloys. Materials Research Society Symposia Proceedings, 2011, 1370, 55.	0.1	5
143	Thermal conductivity of disordered two-dimensional binary alloys. Nanoscale, 2016, 8, 17815-17819.	2.8	5
144	Microstructure of Cu2S nanoprecipitates and its effect on electrical and thermal properties in thermoelectric Cu2Zn0.2Sn0.8S3 ceramics. AIP Advances, 2018, 8, 085105.	0.6	5

#	Article	IF	Citations
145	Intermediate-phase method for computing the natural band offset between two materials with dissimilar structures. Physical Review B, 2018, 97, .	1.1	5
146	Strain Induced Quantum Effect in Semiconductors. Journal of the Physical Society of Japan, 2012, 81, 074712.	0.7	4
147	Evolution of cation ordering and crystal defects controlled by Zn substitutions in Cu2SnS3 ceramics. AIP Advances, 2018, 8, 105322.	0.6	4
148	A chain-type diamine strategy towards strongly anisotropic triiodide of DMEDAÂ·I6. Science China Materials, 2020, 63, 566-574.	3.5	4
149	Searching for Band-Dispersive and Defect-Tolerant Semiconductors from Element Substitution in Topological Materials. Journal of the American Chemical Society, 2022, 144, 4685-4694.	6.6	4
150	Ordered ground state wurtzite alloys from zinc-blende parent compounds. Physical Review B, 2009, 80, .	1.1	3
151	Estimation of gravitational acceleration with quantum optical interferometers. Physical Review A, 2019, 99, .	1.0	3
152	First-principles identification of deep energy levels of sulfur impurities in silicon and their carrier capture cross sections. Journal Physics D: Applied Physics, 2021, 54, 335103.	1.3	3
153	First Report of Meloidogyne graminicola Infecting Chinese Chive in China. Plant Disease, 2019, 103, 2967.	0.7	3
154	Computational prediction of lattice defects in multinary compound semiconductors as photovoltaic materials. Wuli Xuebao/Acta Physica Sinica, 2015, 64, 186102.	0.2	3
155	Strain effect on the diffusion of interstitial Mn in GaAs. Journal of Physics Condensed Matter, 2012, 24, 215801.	0.7	2
156	Cu2ZnSnS4, Cu2ZnSnSe4, and Related Materials. Springer Series in Materials Science, 2016, , 75-103.	0.4	2
157	Structural and electronic properties of the V-V compounds isoelectronic to GaN and isostructural to gray arsenic. Materials Research Express, 2018, 5, 035904.	0.8	2
158	Bandgap Engineering through Halide Doubleâ€Perovskite Alloys: A Highâ€Throughput Firstâ€Principles Study. Physica Status Solidi - Rapid Research Letters, 2021, 15, 2100343.	1.2	2
159	Enhancing neutron radiation resistance of silicon-based semiconductor devices through isotope separation and enrichment. Radiation Effects and Defects in Solids, 2021, 176, 419-430.	0.4	2
160	Orbital-frustration-induced ordering in semiconductor alloys. Physical Review B, 2016, 93, .	1.1	1
161	Defects and dopants in zinc-blende aluminum arsenide: a first-principles study. New Journal of Physics, 2021, 23, 013018.	1.2	1
162	Formation of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mi>Bi</mml:mi><mml:mstyle displaystyle="false" scriptlevel="0"><mml:mtext>â^’</mml:mtext></mml:mstyle><mml:mi>Bi</mml:mi></mml:math> Dimers in Heavily <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mi>Bi</mml:mi></mml:math> -Doped Lead Halide Perovskites: Origin of Carrier Density Saturation. Physical Review Applied, 2022, 17, .	1.5	1

#	Article	IF	Citations
163	Tripleâ€Site Dopantâ€“Defect Complexes in Mgâ€“Hâ€Codoped GaN: Firstâ€Principles Identification. Physica Status Solidi (A) Applications and Materials Science, 2021, 218, 2000723.	0.8	0
164	CuSbSe2 as a Potential Photovoltaic Absorber Material: Studies from Theory to Experiment. , 2016, , .		0