

# Shiyou Chen

## List of Publications by Year in descending order

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164  
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19608

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169  
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169  
docs citations

169  
times ranked

13000  
citing authors

#	ARTICLE	IF	CITATIONS
1	p-type Antimony Selenide via Lead Doping. Solar Rrl, 2022, 6, 2100730.	3.1	12
2	First-principles identification of V <sub>I</sub> +Cu <sub>i</sub> defect cluster in cuprous iodide: origin of red light photoluminescence. Nanotechnology, 2022, 33, 195203.	1.3	7
3	Formation of Bi <sub>2</sub> Dimers in Heavily Bi-Doped Lead Halide Perovskites: Origin of Carrier Density Saturation. Physical Review Applied, 2022, 17, 011101.	1.5	1
4	Evolution of the Interfacial Layer and Its Impact on Electric-Field-Cycling Behaviors in Ferroelectric Hf <sub>1-x</sub> Zr <sub>x</sub> O <sub>2</sub> . ACS Applied Materials & Interfaces, 2022, 14, 11028-11037.	4.0	12
5	Emerging Chalcogenide Thin Films for Solar Energy Harvesting Devices. Chemical Reviews, 2022, 122, 10170-10265.	23.0	81
6	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
7	DASP: Defect and Dopant ab-initio Simulation Package. Journal of Semiconductors, 2022, 43, 042101.	2.0	25
8	Organic-inorganic hybrid perovskite scintillators for mixed field radiation detection. Informa Mater, 2022, 4, .	8.5	25
9	An antibonding valence band maximum enables defect-tolerant and stable GeSe photovoltaics. Nature Communications, 2021, 12, 670.	5.8	58
10	Lead-free hybrid perovskite N(CH <sub>3</sub> ) <sub>4</sub> SnI <sub>3</sub> with robust ferroelectricity induced by large and non-polar N(CH <sub>3</sub> ) <sub>4</sub> <sup>+</sup> molecular cation. Nature Communications, 2021, 12, 637.	5.8	19
11	Defects and dopants in zinc-blende aluminum arsenide: a first-principles study. New Journal of Physics, 2021, 23, 013018.	1.2	1
12	Defect Physics of Ternary Semiconductor P <sub>2</sub> ZnGe with a Defect-Assisted Nonradiative Recombination at Principle Study. Physical Review Applied, 2021, 15, .	1.5	15
13	: A comparative study with Cu <sub>2</sub> ZnSn(S,Se) <sub>4</sub> . Physical Review Materials, 2021, 5, 011101.	0.9	8
14	High Efficiency Cu <sub>2</sub> ZnSn(S,Se) <sub>4</sub> Solar Cells with Shallow Li <sub>Zn</sub> Acceptor Defects Enabled by Solution-Based Li Post-Deposition Treatment. Advanced Energy Materials, 2021, 11, 2003783.	10.2	57
15	Defect Engineering in Earth-Abundant Cu <sub>2</sub> ZnSn(S,Se) <sub>4</sub> Photovoltaic Materials via Ga <sup>3+</sup> Doping for over 12% Efficient Solar Cells. Advanced Functional Materials, 2021, 31, 2010325.	7.8	79
16	Triple-Site Dopant Defect Complexes in Mg-H-Codoped GaN: First-Principles Identification. Physica Status Solidi (A) Applications and Materials Science, 2021, 218, 2000723.	0.8	0
17	Absolute Volume Deformation Potentials of Inorganic ABX <sub>3</sub> Halide Perovskites: The Chemical Trends. Advanced Theory and Simulations, 2021, 4, 2100060.	1.3	11
18	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

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19	Ultrafast non-volatile flash memory based on van der Waals heterostructures. <i>Nature Nanotechnology</i> , 2021, 16, 874-881.	15.6	130
20	Boosting the Electrochemical Performance of All-Solid-State Batteries with Sulfide Li <sub>6</sub> PS <sub>5</sub> Cl Solid Electrolyte Using Li <sub>2</sub> WO <sub>4</sub> -Coated LiCoO <sub>2</sub> Cathode. <i>Advanced Materials Interfaces</i> , 2021, 8, 2100624.	1.9	20
21	Intrinsic Defect Limit to the Growth of Orthorhombic HfO <sub>2</sub> and (Hf,Zr)O <sub>2</sub> with Strong Ferroelectricity: First-Principles Insights. <i>Advanced Functional Materials</i> , 2021, 31, 2104913.	7.8	39
22	More Se Vacancies in Sb <sub>2</sub> Se <sub>3</sub> under Se-Rich Conditions: An Abnormal Behavior Induced by Defect-Correlation in Compensated Compound Semiconductors. <i>Small</i> , 2021, 17, e2102429.	5.2	32
23	Bandgap Engineering through Halide Double-Perovskite Alloys: A High-Throughput First-Principles Study. <i>Physica Status Solidi - Rapid Research Letters</i> , 2021, 15, 2100343.	1.2	2
24	Energy-dependent knock-on damage of organic-inorganic hybrid perovskites under electron beam irradiation: First-principles insights. <i>Applied Physics Letters</i> , 2021, 119, .	1.5	10
25	Role of Polycyclic Aromatic Alkylammonium Cations in Tuning the Electronic Properties and Band Alignment of Two-Dimensional Hybrid Perovskite Semiconductors. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 9754-9760.	2.1	8
26	Enhancing neutron radiation resistance of silicon-based semiconductor devices through isotope separation and enrichment. <i>Radiation Effects and Defects in Solids</i> , 2021, 176, 419-430.	0.4	2
27	A chain-type diamine strategy towards strongly anisotropic triiodide of DMEDA-16. <i>Science China Materials</i> , 2020, 63, 566-574.	3.5	4
28	Intrinsic Defect Limit to the Electrical Conductivity and a Two-Step p-Type Doping Strategy for Overcoming the Efficiency Bottleneck of Sb <sub>2</sub> S <sub>3</sub> -Based Solar Cells. <i>Solar Rrl</i> , 2020, 4, 1900503.	3.1	79
29	Hydrothermal deposition of antimony selenosulfide thin films enables solar cells with 10% efficiency. <i>Nature Energy</i> , 2020, 5, 587-595.	19.8	338
30	Defect Control for 12.5% Efficiency Cu <sub>2</sub> ZnSnSe <sub>4</sub> Kesterite Thin-Film Solar Cells by Engineering of Local Chemical Environment. <i>Advanced Materials</i> , 2020, 32, e2005268.	11.1	133
31	Design of Multifunctional Quaternary Metal-Halide Perovskite Compounds Based on Cation-Anion Co-Ordering. <i>Chemistry of Materials</i> , 2020, 32, 5949-5957.	3.2	10
32	High-stability fluorescent perovskites embedded in PbBrOH triggered by imidazole derivatives in water. <i>Journal of Materials Chemistry C</i> , 2020, 8, 5594-5599.	2.7	24
33	First-principles exploration of defect-pairs in GaN. <i>Journal of Semiconductors</i> , 2020, 41, 032104.	2.0	14
34	Role of Lithium Codoping in Enhancing the Scintillation Yield of Aluminate Garnets. <i>Physical Review Applied</i> , 2020, 13, .	1.5	8
35	Quasi-one-dimensional Sb <sub>2</sub> (S,Se) <sub>3</sub> alloys as bandgap-tunable and defect-tolerant photocatalytic semiconductors. <i>Journal of Chemical Physics</i> , 2020, 153, 014703.	1.2	32
36	Halide Double-Perovskite Light-Emitting Centers Embedded in Lattice-Matched and Coherent Crystalline Matrix. <i>Advanced Functional Materials</i> , 2020, 30, 2000653.	7.8	30

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37	High-throughput first-principles screening of layered magnetic double perovskites Cs <sub>4</sub> MSb <sub>2</sub> X <sub>12</sub> for spintronic applications. Journal of Physics Condensed Matter, 2020, 32, 225705.	0.7	12
38	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
39	Extrinsic dopants in quasi-one-dimensional photovoltaic semiconductor Sb <sub>2</sub> S <sub>3</sub> : A first-principles study. Journal of Applied Physics, 2020, 127, 183101.	1.1	19
40	High-throughput screening and classification of layered di-metal chalcogenides. Nanoscale, 2019, 11, 13924-13933.	2.8	11
41	NaSbSe <sub>2</sub> as a promising light-absorber semiconductor in solar cells: First-principles insights. APL Materials, 2019, 7, 081122.	2.2	11
42	Interfacial engineering to improve Cu <sub>2</sub> ZnSnX <sub>4</sub> (X = S, Se) solar cell efficiency. APL Materials, 2019, 7, .	2.2	19
43	Chemical Trend of Transition-Metal Doping in WSe <sub>2</sub> . Physical Review Applied, 2019, 12, .	1.5	16
44	Polaron-enhanced giant strain effect on defect formation: The case of oxygen vacancies in rutile $\text{TiO}_2$ . Physical Review B, 2019, 99, .	1.1	8
45	Estimation of gravitational acceleration with quantum optical interferometers. Physical Review A, 2019, 99, .	1.0	3
46	Earth-abundant photovoltaic semiconductor NaSbS <sub>2</sub> in the rocksalt-derived structure: A first-principles study. Progress in Natural Science: Materials International, 2019, 29, 322-328.	1.8	8
47	Complicated and Unconventional Defect Properties of the Quasi-One-Dimensional Photovoltaic Semiconductor Sb <sub>2</sub> Se <sub>3</sub> . ACS Applied Materials & Interfaces, 2019, 11, 15564-15572.	4.0	145
48	Low Electron Carrier Concentration Near the p-n Junction Interface: A Fundamental Factor Limiting Short-circuit Current of Cu(In,Ga)Se <sub>2</sub> Solar Cells. Solar Rrl, 2019, 3, 1900057.	3.1	10
49	Rb <sub>4</sub> Ag <sub>2</sub> BiBr <sub>9</sub> : A Lead-Free Visible Light Absorbing Halide Semiconductor with Improved Stability. Inorganic Chemistry, 2019, 58, 4446-4455.	1.9	35
50	Origin of Band-Tail and Deep-Donor States in Cu <sub>2</sub> ZnSnS <sub>4</sub> Solar Cells and Their Suppression through Sn-Poor Composition. Journal of Physical Chemistry Letters, 2019, 10, 7929-7936.	2.1	64
51	Dissociation path competition of radiolysis ionization-induced molecule damage under electron beam illumination. Chemical Science, 2019, 10, 10706-10715.	3.7	19
52	Effective and Noneffective Recombination Center Defects in Cu <sub>2</sub> ZnSnS <sub>4</sub> : Significant Difference in Carrier Capture Cross Sections. Chemistry of Materials, 2019, 31, 826-833.	3.2	72
53	Bulk Assembly of Corrugated 1D Metal Halides with Broadband Yellow Emission. Advanced Optical Materials, 2019, 7, 1801474.	3.6	65
54	In-plane Optical Anisotropy of Low-symmetry 2D GeSe. Advanced Optical Materials, 2019, 7, 1801311.	3.6	68

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55	First Report of <i>Meloidogyne graminicola</i> Infecting Chinese Chive in China. <i>Plant Disease</i> , 2019, 103, 2967.	0.7	3
56	Impact of metal $n$ lone pair on luminescence quantum efficiency in low-dimensional halide perovskites. <i>Physical Review Materials</i> , 2019, 3, .	0.9	60
57	Optoelectronic properties of candidate photovoltaic $\text{Cu}_2\text{PbSiS}_4$ , $\text{Ag}_2\text{PbGeS}_4$ and $\text{KAg}_2\text{SbS}_4$ semiconductors. <i>Journal of Alloys and Compounds</i> , 2018, 746, 405-412.	2.8	10
58	Theoretical study on the kesterite solar cells based on $\text{Cu}_2\text{ZnSn(S,Se)}_4$ and related photovoltaic semiconductors. <i>Chinese Physics B</i> , 2018, 27, 018806.	0.7	10
59	Intrinsic Instability of the Hybrid Halide Perovskite Semiconductor $\text{CH}_3\text{NH}_3\text{PbI}_3$ . <i>Chinese Physics Letters</i> , 2018, 35, 036104.	1.3	154
60	Structural and electronic properties of the V-V compounds isoelectronic to GaN and isostructural to gray arsenic. <i>Materials Research Express</i> , 2018, 5, 035904.	0.8	2
61	Anisotropic in-plane thermal conductivity in multilayer silicene. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2018, 382, 1499-1503.	0.9	6
62	Natural Intermediate Band in I 2 -II-IV-VI4 Quaternary Chalcogenide Semiconductors. <i>Scientific Reports</i> , 2018, 8, 1604.	1.6	15
63	Facile Preparation of Light Emitting Organic Metal Halide Crystals with Near-Unity Quantum Efficiency. <i>Chemistry of Materials</i> , 2018, 30, 2374-2378.	3.2	193
64	First-principles study on the alkali chalcogenide secondary compounds in $\text{Cu}(\text{In,Ga})\text{Se}_2$ and $\text{Cu}_2\text{ZnSn(S,Se)}_4$ thin film solar cells. <i>Journal of Energy Chemistry</i> , 2018, 27, 1140-1150.	7.1	16
65	Evolution of cation ordering and crystal defects controlled by Zn substitutions in $\text{Cu}_2\text{SnS}_3$ ceramics. <i>AIP Advances</i> , 2018, 8, 105322.	0.6	4
66	Broadband Emission in Hybrid Organic-Inorganic Halides of Group 12 Metals. <i>ACS Omega</i> , 2018, 3, 18791-18802.	1.6	70
67	Temperature Dependence of Phonon Modes, Optical Constants, and Optical Band Gap in Two-Dimensional $\text{ReS}_2$ Films. <i>Journal of Physical Chemistry C</i> , 2018, 122, 29464-29469.	1.5	15
68	Organic-Inorganic Layered and Hollow Tin Bromide Perovskite with Tunable Broadband Emission. <i>ACS Applied Materials &amp; Interfaces</i> , 2018, 10, 34363-34369.	4.0	97
69	Efficiency Improvement of $\text{Sb}_2\text{Se}_3$ Solar Cells via Grain Boundary Inversion. <i>ACS Energy Letters</i> , 2018, 3, 2335-2341.	8.8	112
70	Microstructure of $\text{Cu}_2\text{S}$ nanoprecipitates and its effect on electrical and thermal properties in thermoelectric $\text{Cu}_2\text{Zn}_{0.2}\text{Sn}_{0.8}\text{S}_3$ ceramics. <i>AIP Advances</i> , 2018, 8, 085105.	0.6	5
71	Predicting the thermodynamic stability of double-perovskite halides from density functional theory. <i>APL Materials</i> , 2018, 6, .	2.2	42
72	A One-Dimensional Organic Lead Chloride Hybrid with Excitation-Dependent Broadband Emissions. <i>ACS Energy Letters</i> , 2018, 3, 1443-1449.	8.8	124

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73	Hierarchically Structured Thermoelectric Materials in Quaternary System Cu <sup>2+</sup> Zn <sup>2+</sup> Sn <sup>2+</sup> S Featuring a Mosaic-type Nanostructure. ACS Applied Nano Materials, 2018, 1, 2579-2588.	2.4	13
74	The Role of Hydrogen from ALD <sup>Al<sub>2</sub>O<sub>3</sub></sup> in Kesterite Cu <sub>2</sub> ZnSnS <sub>4</sub> Solar Cells: Grain Surface Passivation. Advanced Energy Materials, 2018, 8, 1701940.	10.2	68
75	Unraveling luminescence mechanisms in zero-dimensional halide perovskites. Journal of Materials Chemistry C, 2018, 6, 6398-6405.	2.7	168
76	Intermediate-phase method for computing the natural band offset between two materials with dissimilar structures. Physical Review B, 2018, 97, .	1.1	5
77	Cu <sub>2</sub> ZnSnS <sub>4</sub> solar cells with over 10% power conversion efficiency enabled by heterojunction heat treatment. Nature Energy, 2018, 3, 764-772.	19.8	623
78	Zero-dimensional Cs <sub>4</sub> EuX <sub>6</sub> (X = Br, I) all-inorganic perovskite single crystals for gamma-ray spectroscopy. Journal of Materials Chemistry C, 2018, 6, 6647-6655.	2.7	66
79	Influence of defects and dopants on the photovoltaic performance of Bi <sub>2</sub> S <sub>3</sub> : first-principles insights. Journal of Materials Chemistry A, 2017, 5, 6200-6210.	5.2	97
80	Calculation studies on point defects in perovskite solar cells. Journal of Semiconductors, 2017, 38, 011006.	2.0	20
81	Hydrazine solution processed CuSbSe <sub>2</sub> : Temperature dependent phase and crystal orientation evolution. Solar Energy Materials and Solar Cells, 2017, 168, 112-118.	3.0	23
82	Enhanced Sb <sub>2</sub> Se <sub>3</sub> solar cell performance through theory-guided defect control. Progress in Photovoltaics: Research and Applications, 2017, 25, 861-870.	4.4	154
83	Sodium Passivation of the Grain Boundaries in CuInSe <sub>2</sub> and Cu <sub>2</sub> ZnSnS <sub>4</sub> for High-Efficiency Solar Cells. Advanced Energy Materials, 2017, 7, 1601457.	10.2	56
84	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
85	Large carrier-capture rate of $\text{PbI}_3$ antisite in $\text{Cs}_2\text{PbI}_4$	1.1	13
86	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
87	Comprehensive investigations on charge diffusion physics in SiN-based 3D NAND flash memory through systematical Ab initio calculations. , 2017, , .		18
88	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
89	Chemical instability leads to unusual chemical-potential-independent defect formation and diffusion in perovskite solar cell material CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> . Journal of Materials Chemistry A, 2016, 4, 16975-16981.	5.2	67
90	Hybrid crystalline sp <sup>2</sup> sp <sup>3</sup> carbon as a high-efficiency solar cell absorber. Carbon, 2016, 109, 246-252.	5.4	31

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91	Na $\delta$ -Diffusion Enhanced p $\delta$ -Type Conductivity in Cu(In,Ga)Se <sub>2</sub> : A New Mechanism for Efficient Doping in Semiconductors. <i>Advanced Energy Materials</i> , 2016, 6, 1601191.	10.2	115
92	Thermal conductivity of disordered two-dimensional binary alloys. <i>Nanoscale</i> , 2016, 8, 17815-17819.	2.8	5
93	Giant biquadratic interaction-induced magnetic anisotropy in the iron-based superconductor	1.1	13
94	Orbital-frustration-induced ordering in semiconductor alloys. <i>Physical Review B</i> , 2016, 93, .	1.1	1
95	Self-passivation rule and structure of CdTe $\Gamma$ 3 (112) grain boundaries. <i>Physical Review B</i> , 2016, 93, .	1.1	21
96	Evolution of anatase surface active sites probed by in situ sum-frequency phonon spectroscopy. <i>Science Advances</i> , 2016, 2, e1601162.	4.7	19
97	Deciphering Halogen Competition in Organometallic Halide Perovskite Growth. <i>Journal of the American Chemical Society</i> , 2016, 138, 5028-5035.	6.6	92
98	Cu <sub>2</sub> ZnSnS <sub>4</sub> , Cu <sub>2</sub> ZnSnSe <sub>4</sub> , and Related Materials. <i>Springer Series in Materials Science</i> , 2016, , 75-103.	0.4	2
99	CuSbSe <sub>2</sub> as a Potential Photovoltaic Absorber Material: Studies from Theory to Experiment. , 2016, , .		0
100	Oxygen Vacancy Induced Flat Phonon Mode at FeSe /SrTiO <sub>3</sub> interface. <i>Scientific Reports</i> , 2015, 5, 10011.	1.6	39
101	Engineering Solar Cell Absorbers by Exploring the Band Alignment and Defect Disparity: The Case of Cu $\delta$ - and Ag $\delta$ -Based Kesterite Compounds. <i>Advanced Functional Materials</i> , 2015, 25, 6733-6743.	7.8	284
102	CuSbSe <sub>2</sub> as a Potential Photovoltaic Absorber Material: Studies from Theory to Experiment. <i>Advanced Energy Materials</i> , 2015, 5, 1501203.	10.2	99
103	Thin-film Sb <sub>2</sub> Se <sub>3</sub> photovoltaics with oriented one-dimensional ribbons and benign grain boundaries. <i>Nature Photonics</i> , 2015, 9, 409-415.	15.6	781
104	Antiferromagnetic ground state with pair-checkerboard order in FeSe. <i>Physical Review B</i> , 2015, 91, .	1.1	59
105	Three-step approach for computing band offsets and its application to inorganic perovskites. <i>Physical Review B</i> , 2015, 92, .		
106	Cu-deficiency induced structural transition of Cu <sub>2</sub> xTe. <i>CrystEngComm</i> , 2015, 17, 2878-2885.	1.3	41
107	Cation-Mutation Design of Quaternary Nitride Semiconductors Lattice-Matched to GaN. <i>Chemistry of Materials</i> , 2015, 27, 7757-7764.	3.2	23
108	Indirect-direct band gap transition of two-dimensional arsenic layered semiconductors' cousins of black phosphorus. <i>Science China: Physics, Mechanics and Astronomy</i> , 2015, 58, 1.	2.0	26

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109	Self-Regulation Mechanism for Charged Point Defects in Hybrid Halide Perovskites. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 1791-1794.	7.2	484
110	Inverse design of materials by multi-objective differential evolution. <i>Computational Materials Science</i> , 2015, 98, 51-55.	1.4	55
111	Computational prediction of lattice defects in multinary compound semiconductors as photovoltaic materials. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2015, 64, 186102.	0.2	3
112	Double-hole-induced oxygen dimerization in transition metal oxides. <i>Physical Review B</i> , 2014, 89, .	1.1	26
113	Origin of Reduced Efficiency in Cu(In,Ga)Se <sub>2</sub> Solar Cells With High Ga Concentration: Alloy Solubility Versus Intrinsic Defects. <i>IEEE Journal of Photovoltaics</i> , 2014, 4, 477-482.	1.5	69
114	Phase Stability and Defect Physics of a Ternary ZnSnN <sub>2</sub> Semiconductor: First Principles Insights. <i>Advanced Materials</i> , 2014, 26, 311-315.	11.1	81
115	Bandgap Tunability in Zn(Sn,Ge)N <sub>2</sub> Semiconductor Alloys. <i>Advanced Materials</i> , 2014, 26, 1235-1241.	11.1	75
116	CuSb <sub>2</sub> as a Promising Earth-Abundant Photovoltaic Absorber Material: A Combined Theoretical and Experimental Study. <i>Chemistry of Materials</i> , 2014, 26, 3135-3143.	3.2	278
117	Influence of Defects and Synthesis Conditions on the Photovoltaic Performance of Perovskite Semiconductor CsSn <sub>3</sub> . <i>Chemistry of Materials</i> , 2014, 26, 6068-6072.	3.2	256
118	Design of I <sub>2</sub> and IV <sub>4</sub> Semiconductors through Element Substitution: The Thermodynamic Stability Limit and Chemical Trend. <i>Chemistry of Materials</i> , 2014, 26, 3411-3417.	3.2	128
119	Indolo[3,2,1-jk]carbazole Derivatives-Sensitized Solar Cells: Effect of $\pi$ -Bridges on the Performance of Cells. <i>Journal of Physical Chemistry C</i> , 2014, 118, 14211-14217.	1.5	41
120	Prediction of (TiO <sub>2</sub> ) <sub>x</sub> (Cu <sub>2</sub> O) <sub>y</sub> alloys for efficient photoelectrochemical water splitting. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 1778-1781. <a href="#">Stability and electronic structure of Cu</a>	1.3	17
121	$\text{ZnSnS}_4$ surfaces: First-principles study. <i>Physical Review B</i> , 2013, 88, .	1.1	55
122	Si:WO <sub>3</sub> heterostructure for Z-scheme water splitting: an ab initio study. <i>Journal of Materials Chemistry A</i> , 2013, 1, 1078-1085.	5.2	32
123	Classification of Lattice Defects in the Kesterite Cu <sub>2</sub> ZnSnS <sub>4</sub> and Cu <sub>2</sub> ZnSnSe <sub>4</sub> Earth-Abundant Solar Cell Absorbers. <i>Advanced Materials</i> , 2013, 25, 1522-1539.	11.1	1,210
124	Composition- and Band-Gap-Tunable Synthesis of Wurtzite-Derived Cu <sub>2</sub> ZnSn(S <sub>1-x</sub> Se <sub>x</sub> ) <sub>4</sub> Nanocrystals: Theoretical and Experimental Insights. <i>ACS Nano</i> , 2013, 7, 1454-1463.	7.3	89
125	$\text{Zn(Sn,Ge)Se}$ and Cu <sub>2</sub> ZnSnS <sub>4</sub> surfaces: First-principles study. <i>Physical Review B</i> , 2013, 88, .	1.1	90
126	Pt-Mediated Reversible Reduction and Expansion of CeO <sub>2</sub> in Pt Nanoparticle/Mesoporous CeO <sub>2</sub> Catalyst: In Situ X-ray Spectroscopy and Diffraction Studies under Redox (H <sub>2</sub> and O <sub>2</sub> ) Atmospheres. <i>Journal of Physical Chemistry C</i> , 2013, 117, 26608-26616.	1.5	67



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127	Strain effect on the diffusion of interstitial Mn in GaAs. Journal of Physics Condensed Matter, 2012, 24, 215801.	0.7	2
128	Linearly arranged polytypic CZTSSe nanocrystals. Scientific Reports, 2012, 2, 952.	1.6	45
129	Furfuraldehyde Hydrogenation on Titanium Oxide-Supported Platinum Nanoparticles Studied by Sum Frequency Generation Vibrational Spectroscopy: Acid-Base Catalysis Explains the Molecular Origin of Strong Metal-Support Interactions. Journal of the American Chemical Society, 2012, 134, 14208-14216.	6.6	198
130	Thermodynamic Oxidation and Reduction Potentials of Photocatalytic Semiconductors in Aqueous Solution. Chemistry of Materials, 2012, 24, 3659-3666.	3.2	627
131	Composition dependence of structure and optical properties of Cu <sub>2</sub> ZnSn(S,Se) <sub>4</sub> solid solutions: An experimental study. Journal of Alloys and Compounds, 2012, 511, 129-132.	2.8	181
132	Single-step preparation and characterization of Cu <sub>2</sub> ZnSn(S <sub>x</sub> Se <sub>1-x</sub> ) <sub>4</sub> thin films deposited by pulsed laser deposition method. Journal of Alloys and Compounds, 2012, 529, 34-37.	2.8	68
133	Copper-alloyed ZnS as a p-type transparent conducting material. Physica Status Solidi (A) Applications and Materials Science, 2012, 209, 2101-2107.	0.8	73
134	Strain Induced Quantum Effect in Semiconductors. Journal of the Physical Society of Japan, 2012, 81, 074712.	0.7	4
135	First-principles study on the effective masses of zinc-blend-derived Cu <sub>2</sub> Zn <sup>IV</sup> (IV = Sn, Ge, Si). J. Appl. Phys. 111, 074701 (2012).	1.1	74
136	Abundance of Cu <sub>2</sub> Zn and 2CuZn defect clusters in kesterite solar cells. Applied Physics Letters, 2012, 101, .	1.5	178
137	Temperature dependence of phonon modes, dielectric functions, and interband electronic transitions in Cu <sub>2</sub> ZnSnS <sub>4</sub> semiconductor films. Physical Chemistry Chemical Physics, 2012, 14, 9936.	1.3	38
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163	Band-structure anomalies of the chalcopyrite semiconductors $\text{CuGaX}_2$ versus $\text{AgGaX}_2$ ( $X=\text{S}$ and $\text{Se}$ ) and their alloys. <i>Physical Review B</i> , 2007, 75, .	1.1	132
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