Su-Huai Wei

List of Publications by Year
in descending order

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570 papers	56,511 citations	867 120 h-index	1680 220 g-index
578 all docs	578 docs citations	578 times ranked	44122 citing authors

#	Article	IF	Citations
1	Band gap anomaly in cuprous halides. Computational Materials Science, 2022, 203, 111157.	1.4	7
2	Energetic Cocrystallization as the Most Significant Crystal Engineering Way to Create New Energetic Materials. Crystal Growth and Design, 2022, 22, 954-970.	1.4	20
3	Clarification of the relative magnitude of exciton binding energies in ZnO and SnO2. Applied Physics Letters, 2022, 120, .	1.5	8
4	General Model for Defect Dynamics in Ionizingâ€Irradiated SiO₂â€Si Structures. Small, 2022, 18, e2107516.	5.2	10
5	Designing Ultra-flat Bands in Twisted Bilayer Materials at Large Twist Angles: Theory and Application to Two-Dimensional Indium Selenide. Journal of the American Chemical Society, 2022, 144, 3949-3956.	6.6	19
6	Temperature effect on charge-state transition levels of defects in semiconductors. Physical Review B, 2022, 105, .	1.1	7
7	Origin of Efficiency Enhancement by Lattice Expansion in Hybrid-Perovskite Solar Cells. Physical Review Letters, 2022, 128, 136401.	2.9	28
8	Comment on â€œWideâ€Rangeâ€Tunable pâ€Type Conductivity of Transparent CuI_{1â€x}Br_x Alloyâ€• Advanced Functional Materials, 2022, 32, .	7.8	4
9	Inverse design of stable spinel compounds with high optical absorption via materials genome engineering. Journal of Materials Chemistry A, 2022, 10, 12503-12509.	5.2	3
10	Hydrogenated Cs2AgBiBr6 for significantly improved efficiency of lead-free inorganic double perovskite solar cell. Nature Communications, 2022, 13, .	5.8	109
11	Phase transition behavior of heterostructural alloys: Effects of size mismatch and site preference. Physical Review B, 2022, 105, .	1.1	0
12	Chemical trends in the high thermoelectric performance of the pyrite-type dichalcogenides <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>ZnS</mml:mi><mml:mn>2</mml:mn></mml:msub><mml , and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CdSe</mml:mi><mml:mn>2</mml:mn></mml:msub></m Physical Review B, 2022, 105, .	1.1	6
13	First-principles study of defect control in thin-film solar cell materials. Science China: Physics, Mechanics and Astronomy, 2021, 64, 1.	2.0	17
14	Enhanced performance of Se-alloyed CdTe solar cells: The role of Se-segregation on the grain boundaries. Journal of Applied Physics, 2021, 129, .	1.1	8
15	Approach to achieving a<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>p</mml:mi></mml:math>-type transparent conducting oxide: Doping of bismuth-alloyed<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ga</mml:mi><mml:mn>2</mml:mn></mml:mr mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>with a strongly correlated band edge state. Physical Review B, 2021, 103, .	1.1	24
16	Interface Engineering of Cu(In,Ga)Se₂ Solar Cells by Optimizing Cd- and Zn-Chalcogenide Alloys as the Buffer Layer. ACS Applied Materials & Interfaces, 2021, 13, 15237-15245.	4.0	13
17	Polymorph-Dependent Initial Thermal Decay Mechanism of Energetic Materials: A Case of 1,3,5,7-Tetranitro-1,3,5,7-Tetrazocane. Journal of Physical Chemistry C, 2021, 125, 10057-10067.	1.5	10
18	Electron donation of non-oxide supports boosts O2 activation on nano-platinum catalysts. Nature Communications, 2021, 12, 2741.	5.8	72

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19	Optimization of Doping <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mrow><mml:mi>Cd</mml:mi><mml:mi>Te</mml:mi></mml:mrow></mml:math> Enhancing Magnetic dipole emission in Eu-doped <mml:math	1.5	11
20	xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Sr</mml:mi><mml:mi>M</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> () Tj ETQq0 0 0 rgBT /Overlock 10	1.1	4
21	Origin of the Improved Performance of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mi>Cu</mml:mi><mml:mo		

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37	Designing Dirac semimetals with a honeycomb Na₃Bi-lattice via isovalent cation substitution. Journal of Materials Chemistry C, 2020, 8, 1257-1264.	2.7	4
38	Gamma-ray irradiation-induced oxidation and disproportionation at the amorphous SiO₂/Si interfaces. Journal of Materials Chemistry C, 2020, 8, 17065-17073.	2.7	5
39	Origin of Irradiation Synergistic Effects in Silicon Bipolar Transistors. ACS Applied Electronic Materials, 2020, 2, 3783-3793.	2.0	10
40	Self-Catalyzed Sensitization of CuO Nanowires via a Solvent-free Click Reaction. Langmuir, 2020, 36, 14539-14545.	1.6	6
41	Searching for stable perovskite solar cell materials using materials genome techniques and high-throughput calculations. Journal of Materials Chemistry C, 2020, 8, 12012-12035.	2.7	22
42	Review of the Intermolecular Interactions in Energetic Molecular Cocrystals. Crystal Growth and Design, 2020, 20, 7065-7079.	1.4	64
43	Design of Multifunctional Quinternary Metal-Halide Perovskite Compounds Based on Cationâ€“Anion Co-Ordering. Chemistry of Materials, 2020, 32, 5949-5957.	3.2	10
44	Defect Dynamic Model of the Synergistic Effect in Neutron- and Î³-Ray-Irradiated Silicon NPN Transistors. ACS Applied Materials & Interfaces, 2020, 12, 29993-29998.	4.0	5
45	Unconventional deformation potential and half-metallicity in zigzag nanoribbons of 2D-Xenes. Physical Chemistry Chemical Physics, 2020, 22, 7294-7299.	1.3	4
46	Band-Structure Engineering of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mi>Zn</mml:mi><mml:mi>x</mml:mi></mml:msub><mml:msub><mml:mi>Cd</mml:mi><mml:mi><mml:mn mathvariant="normal">1</mml:mn><mml:mo>−</mml:mo><mml:mi>x</mml:mi></mml:mi></mml:msub><mml:msub><mml:mi>S</mml:mi><mml:mi><mml:mrow><mml:mn mathvariant="normal">1</mml:mn><mml:mo>−</mml:mo><mml:mi>y</mml:mi></mml:mrow></mml:mi></mml:msub><mml:msub><mml:mi>Se</mml:mi><mml:mi>y</mml:mi></mml:msub></mml:math> Alloys. Physical Review Applied, 2020, 13, .	1.5	3
47	Formation of Bloch Flat Bands in Polar Twisted Bilayers without Magic Angles. Physical Review Letters, 2020, 124, 086401.	2.9	52
48	First-principles study of electronic and diffusion properties of intrinsic defects in 4H-SiC. Journal of Applied Physics, 2020, 127, .	1.1	32
49	Strain induced spin-splitting and half-metallicity in antiferromagnetic bilayer silicene under bending. Physical Chemistry Chemical Physics, 2020, 22, 11567-11571.	1.3	6
50	Chemical trend of a Cu impurity in Zn chalcogenides. Physical Review B, 2020, 101, .	1.1	2
51	Realistic dimension-independent approach for charged-defect calculations in semiconductors. Physical Review B, 2020, 101, .	1.1	30
52	Functionalizing Two-Dimensional Materials for Energy Applications. , 2020, , 567-603.		2
53	ToF-SIMS Investigation of the Initial Stages of MeCpPt(CH₃)₃ Adsorption and Decomposition on Nickel Oxide Surfaces: Exploring the Role and Location of the Ligands. Organometallics, 2020, 39, 1024-1034.	1.1	5
54	Theoretical investigation of halide perovskites for solar cell and optoelectronic applications*. Chinese Physics B, 2020, 29, 108401.	0.7	15

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55	Accurate and effective computation of the multi-phonon nonradiative transition. Science China: Physics, Mechanics and Astronomy, 2020, 63, 1.	2.0	0
56	First-principles study of the order-disorder transition and its effects on the optoelectronic property of ABiS2 (A=Na , K). Physical Review Materials, 2020, 4, .	0.9	1
57	The 2019 materials by design roadmap. Journal Physics D: Applied Physics, 2019, 52, 013001.	1.3	236
58	Transition from Positive to Negative Photoconductance in Doped Hybrid Perovskite Semiconductors. Advanced Optical Materials, 2019, 7, 1900865.	3.6	47
59	First-principles study of the band gap tuning and doping control in CdSe_xTe_{1â^'x} alloy for high efficiency solar cell*. Chinese Physics B, 2019, 28, 086106.	0.7	50
60	Revisit of the band gaps of rutile SnO₂ and TiO₂: a first-principles study. Journal of Semiconductors, 2019, 40, 092101.	2.0	24
61	Nanowire Quantum Dot Surface Engineering for High Temperature Single Photon Emission. ACS Nano, 2019, 13, 13492-13500.	7.3	22
62	Achieving High Volumetric Lithium Storage Capacity in Compact Carbon Materials with Controllable Nitrogen Doping. Advanced Functional Materials, 2019, 29, 1807441.	7.8	39
63	Origin of High- T_C Ferromagnetism in Isovalent-Doped III-V Semiconductors. Physical Review Applied, 2019, 11, .	1.5	10
64	UV-ozone induced surface passivation to enhance the performance of Cu2ZnSnS4 solar cells. Solar Energy Materials and Solar Cells, 2019, 200, 109892.	3.0	13
65	Alloy-induced phase transition and enhanced photovoltaic performance: the case of Cs₃Bi₂I_{9â^'x}Br_x perovskite solar cells. Journal of Materials Chemistry A, 2019, 7, 8818-8825.	5.2	87
66	Mechanism of Synergistic Effects of Neutron- and Gamma-Ray-Radiated PNP Bipolar Transistors. ACS Applied Electronic Materials, 2019, 1, 538-547.	2.0	13
67	Origin of Deep <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mi>Be</mml:mi></mml:math> Acceptor Levels in Nitride Semiconductors: The Roles of Chemical and Strain Effects. Physical Review Applied, 2019, 11, .	1.5	17
68	Formation of DY center as n-type limiting defects in octahedral semiconductors: the case of Bi-doped hybrid halide perovskites. Journal of Materials Chemistry C, 2019, 7, 4230-4234.	2.7	41
69	Materials Design of Solar Cell Absorbers Beyond Perovskites and Conventional Semiconductors via Combining Tetrahedral and Octahedral Coordination. Advanced Materials, 2019, 31, e1806593.	11.1	48
70	Origin of the anomalous trends in band alignment of GaX/ZnGeX₂ (X = N, P, As, Sb) heterojunctions. Journal of Semiconductors, 2019, 40, 042102.	2.0	10
71	Hole-Induced Spontaneous Mutual Annihilation of Dislocation Pairs. Journal of Physical Chemistry Letters, 2019, 10, 7421-7425.	2.1	0
72	A systematic study of the negative thermal expansion in zinc-blende and diamond-like semiconductors. New Journal of Physics, 2019, 21, 123015.	1.2	10

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73	Stable Bandgap-Tunable Hybrid Perovskites with Alloyed Pbâ€“Ba Cations for High-Performance Photovoltaic Applications. Journal of Physical Chemistry Letters, 2019, 10, 59-66.	2.1	44
74	The Coulomb interaction in van der Waals heterostructures. Science China: Physics, Mechanics and Astronomy, 2019, 62, 1.	2.0	25
75	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
76	Enabling visible-light absorption and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>p</mml:mi></mml:math> -type doping in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:msub><mml:mi>In</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:math> by adding Bi. Physical Review Materials, 2019, 3, .	0.9	7
77	Design of p -type transparent conductors from inverted band structure: The case of inorganic metal halide perovskites. Physical Review Materials, 2019, 3, .	0.9	20
78	Ab-initio assessment of new sulfo-iodide compounds as candidate top-cell materials for silicon-based multi-junction tandem solar cells. , 2019, , .		0
79	Intrinsic Instability of the Hybrid Halide Perovskite Semiconductor CH ₃ NH ₃ PbI ₃ [*]. Chinese Physics Letters, 2018, 35, 036104.	1.3	154
80	Modulation of electronic and magnetic properties of edge hydrogenated armchair phosphorene nanoribbons by transition metal adsorption. Physical Chemistry Chemical Physics, 2018, 20, 12916-12922.	1.3	10
81	Tuning the optical bandgap in multi-cation compound transparent conducting-oxides: The examples of In2ZnO4 and In4Sn3O12. Journal of Applied Physics, 2018, 123, .	1.1	3
82	Design of nâ€Type Transparent Conducting Oxides: The Case of Transition Metal Doping in In₂O₃. Advanced Electronic Materials, 2018, 4, 1700553.	2.6	58
83	Comment on â€œFundamental Resolution of Difficulties in the Theory of Charged Point Defects in Semiconductorsâ€• Physical Review Letters, 2018, 120, 039601.	2.9	7
84	Manipulation of cation combinations and configurations of halide double perovskites for solar cell absorbers. Journal of Materials Chemistry A, 2018, 6, 1809-1815.	5.2	85
85	CsCu₅Se₃: A Copper-Rich Ternary Chalcogenide Semiconductor with Nearly Direct Band Gap for Photovoltaic Application. Chemistry of Materials, 2018, 30, 1121-1126.	3.2	30
86	First-principles study of alloying effects on fluorine incorporation in Al_xGa_{1â^’x}N alloys. Journal Physics D: Applied Physics, 2018, 51, 065108.	1.3	10
87	Origin of charge compensation and its effect on the stability of oxide cathodes for Li-ion batteries: The case of orthosilicates. Electrochimica Acta, 2018, 270, 409-416.	2.6	10
88	Band Structure Engineering of Cs₂AgBiBr₆ Perovskite through Orderâ€“Disordered Transition: A First-Principle Study. Journal of Physical Chemistry Letters, 2018, 9, 31-35.	2.1	121
89	Highly-anisotropic optical and electrical properties in layered SnSe. Nano Research, 2018, 11, 554-564.	5.8	114
90	Magnetic origin of phase stability in cubic Î³-MoN. Applied Physics Letters, 2018, 113, 221901.	1.5	6

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91	Band structure engineering and defect control of oxides for energy applications. Chinese Physics B, 2018, 27, 117104.	0.7	17
92	Unified theory of direct or indirect band-gap nature of conventional semiconductors. Physical Review B, 2018, 98, .	1.1	60
93	Photocorrosion-Limited Maximum Efficiency of Solar Photoelectrochemical Water Splitting. Physical Review Applied, 2018, 10, .	1.5	44
94	Functionalizing Two-Dimensional Materials for Energy Applications. , 2018, , 1-37.		0
95	Distinct Excitonic Circular Dichroism between Wurtzite and Zincblende CdSe Nanoplatelets. Nano Letters, 2018, 18, 6665-6671.	4.5	68
96	Atomic-Ordering-Induced Quantum Phase Transition between Topological Crystalline Insulator and Z 2 Topological Insulator. Chinese Physics Letters, 2018, 35, 057301.	1.3	6
97	High-throughput screening of chalcogenide single perovskites by first-principles calculations for photovoltaics. Journal Physics D: Applied Physics, 2018, 51, 474003.	1.3	50
98	Preface for Special Topic: Earth abundant materials in solar cells. APL Materials, 2018, 6, .	2.2	2
99	Origin of the stability of two-dimensional perovskites: a first-principles study. Journal of Materials Chemistry A, 2018, 6, 14949-14955.	5.2	79
100	Interface Engineering of Graphene/CH₃NH₃PbI₃ Heterostructure for Novel pâ€“iâ€“n Structural Perovskites Solar Cells. Journal of Physical Chemistry C, 2018, 122, 17228-17237.	1.5	22
101	Influence of defects on the thermoelectricity in SnSe: A comprehensive theoretical study. Physical Review B, 2018, 97, .	1.1	53
102	The stabilization mechanism and size effect of nonpolar-to-polar crystallography facet tailored ZnO nano/micro rods via a top-down strategy. Physical Chemistry Chemical Physics, 2018, 20, 18455-18462.	1.3	3
103	Design of Lead-Free Inorganic Halide Perovskites for Solar Cells via Cation-Transmutation. Journal of the American Chemical Society, 2017, 139, 2630-2638.	6.6	714
104	High Performance Electrocatalytic Reaction of Hydrogen and Oxygen on Ruthenium Nanoclusters. ACS Applied Materials & Interfaces, 2017, 9, 3785-3791.	4.0	108
105	Optical and fundamental band gaps disparity in transparent conducting oxides: new findings for the $mathbf{I}{{mathbf{n}}_{mathbf{2}}}{{mathbf{O}}_{mathbf{3}}}$ and $mathbf{S}{{mathbf{n}}_{{}}}{{mathbf{O}}_{mathbf{2}}}$ systems. Journal of Physics Condensed Matter, 2017, 29, 085501.	0.7	9
106	Antimony Diffusion in CdTe. IEEE Journal of Photovoltaics, 2017, 7, 870-873.	1.5	11
107	Gas sensing in 2D materials. Applied Physics Reviews, 2017, 4, .	5.5	600
108	Earth-Abundant and Non-Toxic SiX (X = S, Se) Monolayers as Highly Efficient Thermoelectric Materials. Journal of Physical Chemistry C, 2017, 121, 123-128.	1.5	41

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109	Synthesis of Cs2AgSbCl6 and improved optoelectronic properties of Cs2AgSbCl6/TiO2 heterostructure driven by the interface effect for lead-free double perovskites solar cells. Applied Physics Letters, 2017, 111, .	1.5	63
110	Exploring Emerging Photovoltaic Materials Beyond Perovskite: The Case of Skutterudite. Chemistry of Materials, 2017, 29, 9429-9435.	3.2	16
111	Inhomogeneous strain-induced half-metallicity in bent zigzag graphene nanoribbons. Npj Computational Materials, 2017, 3, .	3.5	33
112	Microscopic mechanism of the tunable band gap in potassium-doped few-layer black phosphorus. Physical Review B, 2017, 96, .	1.1	17
113	Self-compensation in arsenic doping of CdTe. Scientific Reports, 2017, 7, 4563.	1.6	59
114	Carrier providers or killers: The case of Cu defects in CdTe. Applied Physics Letters, 2017, 111, 042106.	1.5	22
115	Origin of polymorphism of the two-dimensional group-IV monochalcogenides. Physical Review B, 2017, 96, .	1.1	19
116	Enhanced Electrical and Optoelectronic Characteristics of Few-Layer Type-II SnSe/MoS₂ van der Waals Heterojunctions. ACS Applied Materials & Interfaces, 2017, 9, 42149-42155.	4.0	54
117	Nonisovalent Si-III-V and Si-II-VI alloys: Covalent, ionic, and mixed phases. Physical Review B, 2017, 96, .	1.1	2
118	Prediction of Ideal Topological Semimetals with Triply Degenerate Points in the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>NaCu</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></ Physical Review Letters, 2017, 119, 256402.	2.9	36
119	Notice of Removal Antimony diffusion in CdTe. , 2017, , .		0
120	Air Passivation of Chalcogen Vacancies in Twoâ€Đimensional Semiconductors. Angewandte Chemie, 2016, 128, 977-980.	1.6	15
121	Air Passivation of Chalcogen Vacancies in Twoâ€Đimensional Semiconductors. Angewandte Chemie - International Edition, 2016, 55, 965-968.	7.2	80
122	Polymerization of defect states at dislocation cores in InAs. Journal of Applied Physics, 2016, 119, 045706.	1.1	8
123	Wild band edges: The role of bandgap grading and band-edge fluctuations in high-efficiency chalcogenide devices. , 2016, , .		11
124	Metal compound semiconductors functionalized by polymers and their photosensitive properties. Applied Physics Reviews, 2016, 3, .	5.5	3
125	First-principles study of roles of Cu and Cl in polycrystalline CdTe. Journal of Applied Physics, 2016, 119, .	1.1	44
126	Effect of intermixing at CdS/CdTe interface on defect properties. Applied Physics Letters, 2016, 109, 042105.	1.5	9

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127	Suppress carrier recombination by introducing defects: The case of Si solar cell. Applied Physics Letters, 2016, 108, .	1.5	23
128	Origin of the Distinct Diffusion Behaviors of Cu and Ag in Covalent and Ionic Semiconductors. Physical Review Letters, 2016, 117, 165901.	2.9	25
129	Piezophototronic Effect in Singleâ€Atomicâ€Layer MoS₂ for Strainâ€Gated Flexible Optoelectronics. Advanced Materials, 2016, 28, 8463-8468.	11.1	187
130	Fast self-diffusion of ions in CH₃NH₃PbI₃: the interstiticaly mechanism versus vacancy-assisted mechanism. Journal of Materials Chemistry A, 2016, 4, 13105-13112.	5.2	74
131	Naâ€Diffusion Enhanced pâ€type Conductivity in Cu(In,Ga)Se₂: A New Mechanism for Efficient Doping in Semiconductors. Advanced Energy Materials, 2016, 6, 1601191.	10.2	115
132	Phosphorus Diffusion Mechanisms and Deep Incorporation in Polycrystalline and Single-Crystalline CdTe. Physical Review Applied, 2016, 5, .	1.5	26
133	Review on first-principles study of defect properties of CdTe as a solar cell absorber. Semiconductor Science and Technology, 2016, 31, 083002.	1.0	109
134	Simultaneous band-gap narrowing and carrier-lifetime prolongation of organicâ€“inorganic trihalide perovskites. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 8910-8915.	3.3	269
135	Van der Waals metal-semiconductor junction: Weak Fermi level pinning enables effective tuning of Schottky barrier. Science Advances, 2016, 2, e1600069.	4.7	446
136	Non-Radiative Carrier Recombination Enhanced by Two-Level Process: A First-Principles Study. Scientific Reports, 2016, 6, 21712.	1.6	74
137	Highâ€Performance Hydrogen Evolution from MoS_{2(1â€“x)}P_x Solid Solution. Advanced Materials, 2016, 28, 1427-1432.	11.1	309
138	A Unified Understanding of the Thickness-Dependent Bandgap Transition in Hexagonal Two-Dimensional Semiconductors. Journal of Physical Chemistry Letters, 2016, 7, 597-602.	2.1	100
139	Stabilizing Perovskite Structures by Tuning Tolerance Factor: Formation of Formamidinium and Cesium Lead Iodide Solid-State Alloys. Chemistry of Materials, 2016, 28, 284-292.	3.2	1,606
140	Two-Dimensional SiS Layers with Promising Electronic and Optoelectronic Properties: Theoretical Prediction. Nano Letters, 2016, 16, 1110-1117.	4.5	149
141	Alloy Engineering of Defect Properties in Semiconductors: Suppression of Deep Levels in Transition-Metal Dichalcogenides. Physical Review Letters, 2015, 115, 126806.	2.9	81
142	Origin of and tuning the optical and fundamental band gaps in transparent conducting oxides: The case of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>M</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mrow><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:mrow><mml:mo>(</mml:mo><mml:mi>M</mml:mi><m Physical Review B, 2015, 92, .	1.1	17
143	H-stabilized shallow acceptors in N-doped ZnO. Physical Review B, 2015, 92, .	1.1	23
144	The origin of electronic band structure anomaly in topological crystalline insulator group-IV tellurides. Npj Computational Materials, 2015, 1, .	3.5	38

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145	Surface stability and the selection rules of substrate orientation for optimal growth of epitaxial II-VI semiconductors. Applied Physics Letters, 2015, 107, 141607.	1.5	5
146	Self-regulation of charged defect compensation and formation energy pinning in semiconductors. Scientific Reports, 2015, 5, 16977.	1.6	56
147	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
148	Tunable Polarity Behavior and Selfâ€Driven Photoswitching in pâ€WSe₂/nâ€WS₂ Heterojunctions. Small, 2015, 11, 5430-5438.	5.2	114
149	First-principles Study of Defect Control in Solar Cell Materials. , 2015, , .		0
150	Highly stable two-dimensional silicon phosphides: Different stoichiometries and exotic electronic properties. Physical Review B, 2015, 91, .	1.1	58
151	Period-doubling reconstructions of semiconductor partial dislocations. NPG Asia Materials, 2015, 7, e216-e216.	3.8	12
152	Ordering-induced direct-to-indirect band gap transition in multication semiconductor compounds. Physical Review B, 2015, 91, .	1.1	20
153	Effects of deposition termination on Cu2ZnSnSe4 device characteristics. Thin Solid Films, 2015, 582, 184-187.	0.8	29
154	First-principles multiple-barrier diffusion theory: The case study of interstitial diffusion in CdTe. Physical Review B, 2015, 91, .	1.1	33
155	Stability and electronic structure of the low-Î£grain boundaries in CdTe: a density functional study. New Journal of Physics, 2015, 17, 013027.	1.2	31
156	Device Performance of the Mott Insulator<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>LaVO</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></ a Photovoltaic Material. Physical Review Applied, 2015, 3, .	1.5	73
157	Interlayer coupling and optoelectronic properties of ultrathin two-dimensional heterostructures based on graphene, MoS₂ and WS₂. Journal of Materials Chemistry C, 2015, 3, 5467-5473.	2.7	85
158	Origin of the structural diversity of M2O3 (M = Al, Ga, In). Computational Materials Science, 2015, 104, 35-39.	1.4	2
159	Origin of High Electronic Quality in Structurally Disordered CH₃NH₃PbI₃ and the Passivation Effect of Cl and O at Grain Boundaries. Advanced Electronic Materials, 2015, 1, 1500044.	2.6	175
160	Electronic Structure and Optical Properties of Î±-CH₃NH₃PbBr₃ Perovskite Single Crystal. Journal of Physical Chemistry Letters, 2015, 6, 4304-4308.	2.1	136
161	Enhanced p-type dopability of P and As in CdTe using non-equilibrium thermal processing. Journal of Applied Physics, 2015, 118, .	1.1	60
162	Chemical trends of stability and band alignment of lattice-matched II-VI/III-V semiconductor interfaces. Physical Review B, 2015, 91, .	1.1	21

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