Su-Huai Wei

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/7929600/publications.pdf

Version: 2024-02-01

570 papers	56,511 citations	729 120 h-index	1456 220 g-index
578 all docs	578 docs citations	578 times ranked	38420 citing authors

#	Article	IF	Citations
1	Special quasirandom structures. Physical Review Letters, 1990, 65, 353-356.	2.9	2,702
2	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
3	Defect physics of theCuInSe2chalcopyrite semiconductor. Physical Review B, 1998, 57, 9642-9656.	1.1	1,264
4	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
5	Halide perovskite materials for solar cells: a theoretical review. Journal of Materials Chemistry A, 2015, 3, 8926-8942.	5.2	1,114
6	Origin ofp-type doping difficulty in ZnO:â€ƒThe impurity perspective. Physical Review B, 2002, 66, .	1.1	1,068
7	Electronic properties of random alloys: Special quasirandom structures. Physical Review B, 1990, 42, 9622-9649.	1.1	829
8	Design of Narrow-Gap<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>TiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>: A Passivated Codoping Approach for Enhanced Photoelectrochemical Activity. Physical Review Letters, 2009, 102, 036402.	2.9	728
9	Calculated natural band offsets of all IIâ€“VI and IIIâ€“V semiconductors: Chemical trends and the role of cation d orbitals. Applied Physics Letters, 1998, 72, 2011-2013.	1.5	726
10	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
11	Band Edge Electronic Structure of BiVO₄: Elucidating the Role of the Bi s and V d Orbitals. Chemistry of Materials, 2009, 21, 547-551.	3.2	624
12	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
13	Gas sensing in 2D materials. Applied Physics Reviews, 2017, 4, .	5.5	600
14	Kesterite Thinâ€Film Solar Cells: Advances in Materials Modelling of Cu₂ZnSnS₄. Advanced Energy Materials, 2012, 2, 400-409.	10.2	589
15	Crystal and electronic band structure of Cu2ZnSnX4 (X=S and Se) photovoltaic absorbers: First-principles insights. Applied Physics Letters, 2009, 94, .	1.5	585
16	Doping by Large-Size-Mismatched Impurities: The Microscopic Origin of Arsenic- or Antimony-Dopedp-Type Zinc Oxide. Physical Review Letters, 2004, 92, 155504.	2.9	584
17	Role of metaldstates in II-VI semiconductors. Physical Review B, 1988, 37, 8958-8981.	1.1	578
18	Nature of the Band Gap of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>In</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>Revealed by First-Principles Calculations and X-Ray Spectroscopy. Physical Review Letters, 2008, 100, 167402.	2.9	576

#	Article	IF	Citations
19	Chemical trends of defect formation and doping limit in II-VI semiconductors:â€ƒThe case of CdTe. Physical Review B, 2002, 66, .	1.1	548
20	Predicted band-gap pressure coefficients of all diamond and zinc-blende semiconductors: Chemical trends. Physical Review B, 1999, 60, 5404-5411.	1.1	542
21	Giant and Composition-Dependent Optical Bowing Coefficient in GaAsN Alloys. Physical Review Letters, 1996, 76, 664-667.	2.9	526
22	Local-Density-Functional Calculation of the Pressure-Induced Metallization of BaSe and BaTe. Physical Review Letters, 1985, 55, 1200-1203.	2.9	491
23	Selfâ€Regulation Mechanism for Charged Point Defects in Hybrid Halide Perovskites. Angewandte Chemie - International Edition, 2015, 54, 1791-1794.	7.2	484
24	Effects of Ga addition to CuInSe2 on its electronic, structural, and defect properties. Applied Physics Letters, 1998, 72, 3199-3201.	1.5	482
25	Overcoming the doping bottleneck in semiconductors. Computational Materials Science, 2004, 30, 337-348.	1.4	462
26	Defect physics of the kesterite thin-film solar cell absorber Cu2ZnSnS4. Applied Physics Letters, 2010, 96, .	1.5	454
27	Band offsets and optical bowings of chalcopyrites and Znâ€based IIâ€VI alloys. Journal of Applied Physics, 1995, 78, 3846-3856.	1.1	446
28	Van der Waals metal-semiconductor junction: Weak Fermi level pinning enables effective tuning of Schottky barrier. Science Advances, 2016, 2, e1600069.	4.7	446
29	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 Physical Review B, 2009, 79, .	1.1	413
30	A phenomenological model for systematization and prediction of doping limits in IIâ€“VI and Iâ€“IIIâ€“VI2 compounds. Journal of Applied Physics, 1998, 83, 3192-3196.	1.1	412
31	First-principles calculation of band offsets, optical bowings, and defects in CdS, CdSe, CdTe, and their alloys. Journal of Applied Physics, 2000, 87, 1304-1311.	1.1	406
32	Compositional dependence 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: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:mn>4</mml:mn></mml:mro	1.1	399
33	Origin and Enhancement of Hole-Induced Ferromagnetism in First-Row<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msup><mml:mi>d</mml:mi><mml:mn>0</mml:mn></mml:msup></mml:math>Semiconductors. Physical Review Letters, 2009, 102, 017201.	2.9	392
34	Novel and Enhanced Optoelectronic Performances of Multilayer MoS₂â€“WS₂ Heterostructure Transistors. Advanced Functional Materials, 2014, 24, 7025-7031.	7.8	388
35	First-principles study of native defects in anataseTiO2. Physical Review B, 2006, 73, .	1.1	346
36	Valence band splittings and band offsets of AlN, GaN, and InN. Applied Physics Letters, 1996, 69, 2719-2721.	1.5	322

#	Article	IF	Citations
37	Effects of Na on the electrical and structural properties of CuInSe2. Journal of Applied Physics, 1999, 85, 7214-7218.	1.1	322
38	Bipolar Doping and Band-Gap Anomalies in Delafossite Transparent Conductive Oxides. Physical Review Letters, 2002, 88, 066405.	2.9	314
39	Band structure and fundamental optical transitions in wurtzite AlN. Applied Physics Letters, 2003, 83, 5163-5165.	1.5	310
40	Highâ€Performance Hydrogen Evolution from MoS_{2(1â€“x)}P_x Solid Solution. Advanced Materials, 2016, 28, 1427-1432.	11.1	309
41	Stabilization of Ternary Compounds via Ordered Arrays of Defect Pairs. Physical Review Letters, 1997, 78, 4059-4062.	2.9	303
42	Band structure engineering of semiconductors for enhanced photoelectrochemical water splitting: The case of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msu Physical Review B, 2010, 82, .	1.1	300
43	The state and future prospects of kesterite photovoltaics. Energy and Environmental Science, 2013, 6, 3171.	15.6	294
44	First-principles statistical mechanics of structural stability of intermetallic compounds. Physical Review B, 1991, 44, 512-544.	1.1	286
45	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
46	Origins of band-gap renormalization in degenerately doped semiconductors. Physical Review B, 2008, 78, .	1.1	282
47	Electronic and structural anomalies in lead chalcogenides. Physical Review B, 1997, 55, 13605-13610.	1.1	279
48	Localization and percolation in semiconductor alloys: GaAsN vs GaAsP. Physical Review B, 1996, 54, 17568-17576.	1.1	278
49	Doping of ZnO by group-IB elements. Applied Physics Letters, 2006, 89, 181912.	1.5	275
50	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
51	First-principles calculation of temperature-composition phase diagrams of semiconductor alloys. Physical Review B, 1990, 41, 8240-8269.	1.1	267
52	Predicting the spin-lattice order of frustrated systems from first principles. Physical Review B, 2011, 84, .	1.1	262
53	Theoretical Description of Carrier Mediated Magnetism in Cobalt Doped ZnO. Physical Review Letters, 2008, 100, 256401.	2.9	261
54	First-principles calculation of alloy phase diagrams: The renormalized-interaction approach. Physical Review B, 1989, 40, 3197-3231.	1.1	259

#	Article	IF	Citations
55	Wurtzite-derived polytypes of kesterite and stannite quaternary chalcogenide semiconductors. Physical Review B, 2010, 82, .	1.1	259
56	Influence of Defects and Synthesis Conditions on the Photovoltaic Performance of Perovskite Semiconductor CsSnI₃. Chemistry of Materials, 2014, 26, 6068-6072.	3.2	256
57	Predicting Two-Dimensional Boronâ€“Carbon Compounds by the Global Optimization Method. Journal of the American Chemical Society, 2011, 133, 16285-16290.	6.6	242
58	Bandâ€gap narrowing in ordered and disordered semiconductor alloys. Applied Physics Letters, 1990, 56, 662-664.	1.5	241
59	The 2019 materials by design roadmap. Journal Physics D: Applied Physics, 2019, 52, 013001.	1.3	236
60	Total-energy and band-structure calculations for the semimagneticCd1â^'xMnxTe semiconductor alloy and its binary constituents. Physical Review B, 1987, 35, 2340-2365.	1.1	235
61	Theoretical study of the effects of isovalent coalloying of Bi and N in GaAs. Physical Review B, 2002, 65, .	1.1	235
62	Band gaps and spin-orbit splitting of ordered and disorderedAlxGa1â^'xAsandGaAsxSb1â^'xalloys. Physical Review B, 1989, 39, 3279-3304.	1.1	231
63	Anomalous Alloy Properties in Mixed Halide Perovskites. Journal of Physical Chemistry Letters, 2014, 5, 3625-3631.	2.1	231
64	Nitrogen Solubility and Induced Defect Complexes in Epitaxial GaAs:N. Physical Review Letters, 2001, 86, 1789-1792.	2.9	228
65	Structure stability and carrier localization inCdX(X=S,Se,Te)semiconductors. Physical Review B, 2000, 62, 6944-6947.	1.1	212
66	Localization and anticrossing of electron levels inGaAs1â^'xNxalloys. Physical Review B, 1999, 60, R11245-R11248.	1.1	210
67	Layer-dependent electrical and optoelectronic responses of ReSe2 nanosheet transistors. Nanoscale, 2014, 6, 7226.	2.8	205
68	Microscopic Origin of the Phenomenological Equilibrium â€œDoping Limit Ruleâ€•inn-Type III-V Semiconductors. Physical Review Letters, 2000, 84, 1232-1235.	2.9	204
69	Possible Approach to Overcome the Doping Asymmetry in Wideband Gap Semiconductors. Physical Review Letters, 2007, 98, 135506.	2.9	204
70	Design of shallow acceptors inZnO: First-principles band-structure calculations. Physical Review B, 2006, 74, .	1.1	198
71	Role ofdorbitals in valence-band offsets of common-anion semiconductors. Physical Review Letters, 1987, 59, 144-147.	2.9	196
72	Doping properties of monoclinic BiVO<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></mml:msub></mml:mrow></mml:math>studied by first-principles density-functional theory. Physical Review B, 2011, 83, .	1.1	194

#	Article	IF	Citations
73	Electrically Benign Behavior of Grain Boundaries in Polycrystalline<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>CuInSe</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>Films. Physical Review Letters, 2007, 99, 235504.	2.9	192
74	Revised ab initio natural band offsets of all group IV, II-VI, and III-V semiconductors. Applied Physics Letters, 2009, 94, .	1.5	188
75	Doping asymmetry in wideâ€bandgap semiconductors: Origins and solutions. Physica Status Solidi (B): Basic Research, 2008, 245, 641-652.	0.7	187
76	Piezophototronic Effect in Singleâ€Atomicâ€Layer MoS₂ for Strainâ€Gated Flexible Optoelectronics. Advanced Materials, 2016, 28, 8463-8468.	11.1	187
77	Electronic structure and phase stability of MgO, ZnO, CdO, and related ternary alloys. Physical Review B, 2008, 77, .	1.1	186
78	Fundamental optical transitions in GaN. Applied Physics Letters, 1996, 68, 2784-2786.	1.5	185
79	Effective band gap narrowing of anatase TiO2 by strain along a soft crystal direction. Applied Physics Letters, 2010, 96, .	1.5	185
80	Abundance of CuZnâ€‰+â€‰SnZn and 2CuZnâ€‰+â€‰SnZn defect clusters in kesterite solar cells. Applied Physics Letters, 2012, 101, .	1.5	178
81	Relationships between the band gaps of the zinc-blende and wurtzite modifications of semiconductors. Physical Review B, 1994, 50, 2715-2718.	1.1	175
82	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
83	Resonant hole localization and anomalous optical bowing in InGaN alloys. Applied Physics Letters, 1999, 74, 1842-1844.	1.5	173
84	Spin-Orbit Coupling and Ion Displacements in Multiferroic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>TbMnO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2008, 101, 037209.	2.9	171
85	High thermoelectric performance in copper telluride. NPG Asia Materials, 2015, 7, e210-e210.	3.8	170
86	Structural, magnetic, and electronic properties of the Co-Fe-Al oxide spinel system: Density-functional theory calculations. Physical Review B, 2007, 76, .	1.1	168
87	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"		

#	Article	IF	Citations
91	Calculated spin-orbit splitting of all diamondlike and zinc-blende semiconductors: Effects ofp1â^•2local orbitals and chemical trends. Physical Review B, 2004, 70, .	1.1	152
92	Origin of the unusually large band-gap bowing and the breakdown of the band-edge distribution rule in theSnxGe1â^'xalloys. Physical Review B, 2008, 78, .	1.1	149
93	Two-Dimensional SiS Layers with Promising Electronic and Optoelectronic Properties: Theoretical Prediction. Nano Letters, 2016, 16, 1110-1117.	4.5	149
94	Origin of the Structural and Magnetic Anomalies of the Layered Compound<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>SrFeO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>: A Density Functional Investigation. Physical Review Letters, 2008, 100, 167207.	2.9	148
95	First-principles calculations of the phase diagrams of noble metals: Cu-Au, Cu-Ag, and Ag-Au. Physical Review B, 1987, 36, 4163-4185.	1.1	147
96	Ground-state structures and the random-state energy of the Madelung lattice. Physical Review B, 1990, 42, 11388-11391.	1.1	147
97	Pseudopotential plane-wave calculations for ZnS. Physical Review B, 1991, 43, 2213-2217.	1.1	144
98	Optical properties of zinc-blende semiconductor alloys: Effects of epitaxial strain and atomic ordering. Physical Review B, 1994, 49, 14337-14351.	1.1	143
99	Phase control of CuxTe film and its effects on CdS/CdTe solar cell. Thin Solid Films, 2007, 515, 5798-5803.	0.8	143
100	Ab initioall-electron calculation of absolute volume deformation potentials of IV-IV, III-V, and II-VI semiconductors: The chemical trends. Physical Review B, 2006, 73, .	1.1	140
101	Dependence of the optical properties of semiconductor alloys on the degree of longâ€range order. Applied Physics Letters, 1993, 62, 1937-1939.	1.5	139
102	Hydrogen passivation effect in nitrogen-doped ZnO thin films. Applied Physics Letters, 2005, 86, 122107.	1.5	139
103	Linearized augmented-plane-wave calculation of the electronic structure and total energy of tungsten. Physical Review B, 1985, 32, 7792-7797.	1.1	137
104	Composition dependence of interband transition intensities in GaPN, GaAsN, and GaPAs alloys. Physical Review B, 1997, 56, 10233-10240.	1.1	137
105	Realizing a SnO2-based ultraviolet light-emitting diode via breaking the dipole-forbidden rule. NPG Asia Materials, 2012, 4, e30-e30.	3.8	137
106	Towards Direct-Gap Silicon Phases by the Inverse Band Structure Design Approach. Physical Review Letters, 2013, 110, 118702.	2.9	136
107	Electronic Structure and Optical Properties of Î±-CH₃NH₃PbBr₃ Perovskite Single Crystal. Journal of Physical Chemistry Letters, 2015, 6, 4304-4308.	2.1	136
108	Electronic, structural, and magnetic effects of 3d transition metals in hematite. Journal of Applied Physics, 2010, 107, .	1.1	135

#	Article	IF	Citations
109	Effective Control of the Charge and Magnetic States of Transition-Metal Atoms on Single-Layer Boron Nitride. Physical Review Letters, 2012, 108, 206802.	2.9	135
110	Engineering Grain Boundaries in Cu₂ZnSnSe₄ for Better Cell Performance: A Firstâ€Principle Study. Advanced Energy Materials, 2014, 4, 1300712.	10.2	135
111	Phenomenological band structure model of magnetic coupling in semiconductors. Solid State Communications, 2006, 138, 353-358.	0.9	134
112	Double-Hole-Mediated Coupling of Dopants and Its Impact on Band Gap Engineering in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>TiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2011, 106, 066801.	2.9	134
113	Band-structure anomalies of the chalcopyrite semiconductorsCuGaX2versusAgGaX2(X=Sand Se) and their alloys. Physical Review B, 2007, 75, .	1.1	132
114	Origin of the Variation of Exciton Binding Energy in Semiconductors. Physical Review Letters, 2013, 110, 016402.	2.9	132
115	Surface Energy and the Common Dangling Bond Rule for Semiconductors. Physical Review Letters, 2004, 92, 086102.	2.9	130
116	Design of I₂â€“IIâ€“IVâ€“VI₄ Semiconductors through Element Substitution: The Thermodynamic Stability Limit and Chemical Trend. Chemistry of Materials, 2014, 26, 3411-3417.	3.2	128
117	Theoretical study of the band-gap anomaly of InN. Journal of Applied Physics, 2005, 97, 033707.	1.1	124
118	Dependence of the Minority-Carrier Lifetime on the Stoichiometry of CdTe Using Time-Resolved Photoluminescence and First-Principles Calculations. Physical Review Letters, 2013, 111, 067402.	2.9	124
119	Structure-derived electronic and optical properties of transparent conducting oxides. Physical Review B, 2005, 71, .	1.1	123
120	Substitutional diatomic molecules NO, NC, CO, N2, and O2: Their vibrational frequencies and effects on p doping of ZnO. Applied Physics Letters, 2005, 86, 211910.	1.5	121
121	Strong Dzyaloshinskii-Moriya Interaction and Origin of Ferroelectricity in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Cu</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi>OSeO</mml:mi><mml:mi><m Physical Review Letters, 2012, 109, 107203.	2.9	121
122	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
123	Electron-induced stabilization of ferromagnetism inGa1â^'xGdxN. Physical Review B, 2005, 72, .	1.1	120
124	â€œNarrowâ€•Graphene Nanoribbons Made Easier by Partial Hydrogenation. Nano Letters, 2009, 9, 4025-4030.	4.5	120
125	Carrier density and compensation in semiconductors with multiple dopants and multiple transition energy levels: Case of Cu impurities in CdTe. Physical Review B, 2011, 83, .	1.1	118
126	Origin of the superior conductivity of perovskite Ba(Sr)SnO3. Applied Physics Letters, 2013, 102, .	1.5	116

#	Article	IF	Citations
127	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
128	Tunable Polarity Behavior and Selfâ€Driven Photoswitching in pâ€WSe₂/nâ€WS₂ Heterojunctions. Small, 2015, 11, 5430-5438.	5.2	114
129	Highly-anisotropic optical and electrical properties in layered SnSe. Nano Research, 2018, 11, 554-564.	5.8	114
130	Native defect-induced multifarious magnetism in nonstoichiometric cuprous oxide: First-principles study of bulk and surface properties of<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:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>O. Physical Review B, 2009, 79, .	1.1	109
131	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
132	Hydrogenated Cs2AgBiBr6 for significantly improved efficiency of lead-free inorganic double perovskite solar cell. Nature Communications, 2022, 13, .	5.8	109
133	High Performance Electrocatalytic Reaction of Hydrogen and Oxygen on Ruthenium Nanoclusters. ACS Applied Materials & Interfaces, 2017, 9, 3785-3791.	4.0	108
134	Ordering of isovalent intersemiconductor alloys. Physical Review B, 1988, 38, 6338-6341.	1.1	106
135	Long-range order in binary late-transition-metal alloys. Physical Review Letters, 1991, 66, 1753-1756.	2.9	105
136	Crystal and electronic structures of CuxS solar cell absorbers. Applied Physics Letters, 2012, 100, .	1.5	105
137	Electronic structure and phase stability of LiZnAs: A half ionic and half covalent tetrahedral semiconductor. Physical Review Letters, 1986, 56, 528-531.	2.9	104
138	Band offsets at the CdS/CuInSe2heterojunction. Applied Physics Letters, 1993, 63, 2549-2551.	1.5	103
139	Fingerprints of CuPt ordering in III-V semiconductor alloys: Valence-band splittings, band-gap reduction, and x-ray structure factors. Physical Review B, 1998, 57, 8983-8988.	1.1	103
140	Effect of Copassivation of Cl and Cu on CdTe Grain Boundaries. Physical Review Letters, 2008, 101, 155501.	2.9	103
141	â€œMajority Representationâ€•of Alloy Electronic States. Physical Review Letters, 1998, 80, 4725-4728.	2.9	101
142	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
143	Interactions between nitrogen, hydrogen, and gallium vacancies inGaAs1â^'xNxalloys. Physical Review B, 2003, 67, .	1.1	99
144	Breakdown of the band-gap-common-cation rule:â€,â€,The origin of the small band gap of InN. Physical Review B, 2003, 67, .	1.1	97

#	Article	IF	Citations
145	Strain-Enhanced Doping in Semiconductors: Effects of Dopant Size and Charge State. Physical Review Letters, 2010, 105, 195503.	2.9	97
146	Effects of Hydrogen on the Electronic Properties of Dilute GaAsN Alloys. Physical Review Letters, 2002, 89, 086403.	2.9	95
147	Density-functional theory study of the effects of atomic impurity on the band edges of monoclinic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>WO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:ms Physical Review B, 2008, 77, .	1.1	93
148	Electronic structure of ZnO:GaN compounds: Asymmetric bandgap engineering. Physical Review B, 2008, 78, .	1.1	93
149	Evolution of alloy properties with long-range order. Physical Review Letters, 1992, 69, 3766-3769.	2.9	91
150	Disorder effects on the density of states of the II-VI semiconductor alloysHg0.5Cd0.5Te,Cd0.5Zn0.5Te, andHg0.5Zn0.5Te. Physical Review B, 1991, 43, 1662-1677.	1.1	90
151	First-principles calculation of the order-disorder transition in chalcopyrite semiconductors. Physical Review B, 1992, 45, 2533-2536.	1.1	90
152	Interplay between Order and Disorder in the High Performance of Amorphous Transparent Conducting Oxides. Chemistry of Materials, 2009, 21, 5119-5124.	3.2	90
153	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
154	Electronic structure of ordered and disorderedCu3Au andCu3Pd. Physical Review B, 1992, 45, 10314-10330.	1.1	89
155	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
156	Vibrational and crystalline properties of polymorphicCuInC2(C=Se,S)chalcogenides. Physical Review B, 2005, 71, .	1.1	86
157	Origin of Long-Range Ferromagnetic Ordering in Metalâ€“Organic Frameworks with Antiferromagnetic Dimeric-Cu(II) Building Units. Journal of the American Chemical Society, 2012, 134, 17286-17290.	6.6	86
158	First-principles study of transparentp-type conductiveSrCu2O2and related compounds. Physical Review B, 2002, 65, .	1.1	85
159	Energetics and electronic structure of stacking faults in ZnO. Physical Review B, 2004, 70, .	1.1	85
160	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
161	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
162	Defect properties of CuInSe2 and CuGaSe2. Journal of Physics and Chemistry of Solids, 2005, 66, 1994-1999.	1.9	84

#	Article	IF	Citations
163	Ab initio calculation of hydrostatic absolute deformation potential of semiconductors. Applied Physics Letters, 2006, 88, 042104.	1.5	81
164	Alloy Engineering of Defect Properties in Semiconductors: Suppression of Deep Levels in Transition-Metal Dichalcogenides. Physical Review Letters, 2015, 115, 126806.	2.9	81
165	Air Passivation of Chalcogen Vacancies in Twoâ€Đimensional Semiconductors. Angewandte Chemie - International Edition, 2016, 55, 965-968.	7.2	80
166	First-principles simulated-annealing study of phase transitions and short-range order in transition-metal and semiconductor alloys. Physical Review B, 1994, 50, 6642-6661.	1.1	79
167	Band structure and stability of zinc-blende-based semiconductor polytypes. Physical Review B, 1999, 59, R2478-R2481.	1.1	79
168	Design of Shallow Donor Levels in Diamond by Isovalent-Donor Coupling. Physical Review Letters, 2003, 91, 126406.	2.9	79
169	Strain control of magnetism in graphene decorated by transition-metal atoms. Physical Review B, 2011, 84, .	1.1	79
170	Origin of the stability of two-dimensional perovskites: a first-principles study. Journal of Materials Chemistry A, 2018, 6, 14949-14955.	5.2	79
171	Oxygen-vacancy mediated adsorption and reactions of molecular oxygen on theZnO(101Â¯0)surface. Physical Review B, 2005, 72, .	1.1	78
172	Band-gap bowing coefficients in large size-mismatched II-VI alloys: first-principles calculations. Physical Review B, 2006, 74, .	1.1	78
173	Kesterite Successes, Ongoing Work, and Challenges: A Perspective From Vacuum Deposition. IEEE Journal of Photovoltaics, 2013, 3, 439-445.	1.5	78
174	Structural motifs in oxidized graphene: A genetic algorithm study based on density functional theory. Physical Review B, 2010, 82, .	1.1	77
175	Electronic structure of ultrathin (GaAs)n(AlAs)n[001] superlattices and the Ga0.5Al0.5As alloy. Journal of Applied Physics, 1988, 63, 5794-5804.	1.1	76
176	Study of defect levels in CdTe using thermoelectric effect spectroscopy. Journal of Electronic Materials, 2006, 35, 1333-1340.	1.0	76
177	Electronic, Energetic, and Chemical Effects of Intrinsic Defects and Fe-Doping of CoAl₂O₄: A DFT+UStudy. Journal of Physical Chemistry C, 2008, 112, 12044-12050.	1.5	75
178	Polymorphism in CuInS2 epilayers: Origin of additional Raman modes. Applied Physics Letters, 2002, 80, 562-564.	1.5	74
179	Origin of electronic and optical trends in ternary<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>In</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:ms conducting oxides<mml:math xmlns . Physical Review B, 2009, 79, .	1.1	74
180	Implications of the formation of small polarons in Li<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>O<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>for Li-air batteries. Physical Review B, 2012, 85, .	1.1	74

#	Article	IF	Citations
181	First-principles study on the effective masses of zinc-blend-derived Cu2Znâ^'IVâ^'VI4 (IVâ€‰=â€‰Sn, Ge, Si) Tj ETQq1 1 0.784	1.1	74
182	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
183	Non-Radiative Carrier Recombination Enhanced by Two-Level Process: A First-Principles Study. Scientific Reports, 2016, 6, 21712.	1.6	74
184	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
185	Alloy-Stabilized Semiconducting and Magnetic Zinc-Blende Phase of MnTe. Physical Review Letters, 1986, 56, 2391-2394.	2.9	72
186	A Novel Codoping Approach for Enhancing the Performance of LiFePO₄ Cathodes. Advanced Energy Materials, 2012, 2, 1028-1032.	10.2	72
187	Impact of bulk properties and local secondary phases on the Cu2(Zn,Sn)Se4 solar cells open-circuit voltage. Solar Energy Materials and Solar Cells, 2015, 133, 119-125.	3.0	72
188	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
189	Electron donation of non-oxide supports boosts O2 activation on nano-platinum catalysts. Nature Communications, 2021, 12, 2741.	5.8	72
190	Stability of coherently strained semiconductor superlattices. Physical Review Letters, 1990, 64, 36-39.	2.9	71
191	Electronic origins of the magnetic phase transitions in zinc-blende Mn chalcogenides. Physical Review B, 1993, 48, 6111-6115.	1.1	71
192	Superhard PseudocubicBC2NSuperlattices. Physical Review Letters, 2007, 98, 015502.	2.9	71
193	InAsSb/InAs: A type-I or a type-II band alignment. Physical Review B, 1995, 52, 12039-12044.	1.1	70
194	Strain relaxation and band-gap tunability in ternary<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>In</mml:mtext></mml:mrow><mml:mi>x</mml:mi></mml:msub> Physical Review B, 2008, 78, .	1.1	69
195	Group-IIIA versus IIIB delafossites: Electronic structure study. Physical Review B, 2009, 80, .	1.1	69
196	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
197	Chemical Functionalization of Silicene: Spontaneous Structural Transition and Exotic Electronic Properties. Physical Review Letters, 2013, 111, 145502.	2.9	68
198	Distinct Excitonic Circular Dichroism between Wurtzite and Zincblende CdSe Nanoplatelets. Nano Letters, 2018, 18, 6665-6671.	4.5	68

#	Article	IF	Citations
199	Tuning the Fermi level beyond the equilibrium doping limit through quenching: The case of CdTe. Physical Review B, 2014, 90, .	1.1	66
200	Multiband coupling and electronic structure of(InAs)n/(GaSb)nsuperlattices. Physical Review B, 1999, 60, 5590-5596.	1.1	65
201	Thermodynamic instability of ultrathin semiconductor superlattices: The (001) (GaAs)1(AlAs)1structure. Physical Review Letters, 1987, 58, 1123-1126.	2.9	64
202	Review of the Intermolecular Interactions in Energetic Molecular Cocrystals. Crystal Growth and Design, 2020, 20, 7065-7079.	1.4	64
203	Instability of the ideal tungsten (001) surface. Physical Review Letters, 1986, 57, 3292-3295.	2.9	63
204	Stability and electronic structure of ultrathin [001] (GaAs)m(AlAs)msuperlattices. Physical Review B, 1988, 37, 1342-1363.	1.1	63
205	Rules of thumb for formation for the Homologous<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>In</mml:mi><mml:mi>M</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mo stretchy="false">(</mml:mo><mml:mi>ZnO</mml:mi><mml:msub><mml:mo) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 487 Td (sti	2.9	63
206	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
207	Electronic structure of randomAg0.5Pd0.5andAg0.5Au0.5alloys. Physical Review B, 1991, 44, 10470-10484.	1.1	62
208	Trends in band-gap pressure coefficients in chalcopyrite semiconductors. Physical Review B, 1998, 58, R1710-R1713.	1.1	62
209	Dielectric functions and electronic band structure of lead zirconate titanate thin films. Journal of Applied Physics, 2005, 98, 094108.	1.1	62
210	Stability and electronic structures of CuxTe. Applied Physics Letters, 2007, 91, .	1.5	61
211	Impurity effects in ZnO and nitrogen-doped ZnO thin films fabricated by MOCVD. Journal of Crystal Growth, 2006, 287, 94-100.	0.7	60
212	Ternary cobalt spinel oxides for solar driven hydrogen production: Theory and experiment. Energy and Environmental Science, 2009, 2, 774.	15.6	60
213	Structures of [Ag₇(SR)₄]^{â^'}and [Ag₇(DMSA)₄]^{â^'}. Journal of the American Chemical Society, 2010, 132, 7355-7360.	6.6	60
214	Band structure engineering of multinary chalcogenide topological insulators. Physical Review B, 2011, 83, .	1.1	60
215	Enhanced p-type dopability of P and As in CdTe using non-equilibrium thermal processing. Journal of Applied Physics, 2015, 118, .	1.1	60
216	Unified theory of direct or indirect band-gap nature of conventional semiconductors. Physical Review B, 2018, 98, .	1.1	60

#	Article	IF	Citations
217	Epitaxy-induced structural phase transformations. Physical Review B, 1988, 38, 10124-10127.	1.1	59
218	Proposal for IIIâ€V ordered alloys with infrared band gaps. Applied Physics Letters, 1991, 58, 2684-2686.	1.5	59
219	Origin of insulating behavior of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>p</mml:mi></mml:math>-type<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>LaAlO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> Polarization induced asymmetric distribution of oxygen va. Physical Review B, 2010, 82, .	1.1	59
220	Self-compensation in arsenic doping of CdTe. Scientific Reports, 2017, 7, 4563.	1.6	59
221	Observation and first-principles calculation of buried wurtzite phases in zinc-blende CdTe thin films. Applied Physics Letters, 2000, 77, 1461-1463.	1.5	58
222	Highly stable two-dimensional silicon phosphides: Different stoichiometries and exotic electronic properties. Physical Review B, 2015, 91, .	1.1	58
223	Design of nâ€Type Transparent Conducting Oxides: The Case of Transition Metal Doping in In₂O₃. Advanced Electronic Materials, 2018, 4, 1700553.	2.6	58
224	First-Principles Study of Doping Limits of CdTe. Physica Status Solidi (B): Basic Research, 2002, 229, 305-310.	0.7	56
225	Origin of antiferromagnetism in CoO: A density functional theory study. Applied Physics Letters, 2010, 96, .	1.5	56
226	Theoretical study of corundum as an ideal gate dielectric material for graphene transistors. Physical Review B, 2011, 84, .	1.1	56
227	First-Principles Theory of Electrochemical Capacitance of Nanostructured Materials: Dipole-Assisted Subsurface Intercalation of Lithium in Pseudocapacitive TiO₂ Anatase Nanosheets. Journal of Physical Chemistry C, 2011, 115, 4909-4915.	1.5	56
228	Self-regulation of charged defect compensation and formation energy pinning in semiconductors. Scientific Reports, 2015, 5, 16977.	1.6	56
229	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
230	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
231	Self-doping of cadmium stannate in the inverse spinel structure. Applied Physics Letters, 2002, 80, 1376-1378.	1.5	54
232	Enhanced Ferromagnetic Stability in Cu Doped Passivated GaN Nanowires. Nano Letters, 2008, 8, 1825-1829.	4.5	54
233	Band crossing in isovalent semiconductor alloys with large size mismatch: First-principles calculations of the electronic structure of Bi and N incorporated GaAs. Physical Review B, 2010, 82, .	1.1	54
234	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

#	Article	IF	Citations
235	Off-center atomic displacements in zinc-blende semiconductor. Physical Review Letters, 1993, 70, 1639-1642.	2.9	53
236	Optical properties of (GeTe, Sb2Te3) pseudobinary thin films studied with spectroscopic ellipsometry. Applied Physics Letters, 2008, 93, .	1.5	53
237	Kesterites and Chalcopyrites: A Comparison of Close Cousins. Materials Research Society Symposia Proceedings, 2011, 1324, 97.	0.1	53
238	Influence of defects on the thermoelectricity in SnSe: A comprehensive theoretical study. Physical Review B, 2018, 97, .	1.1	53
239	Novel Approach to Tuning the Physical Properties of Organic-Inorganic Hybrid Semiconductors. Physical Review Letters, 2006, 96, 026405.	2.9	52
240	Multi-component transparent conducting oxides: progress in materials modelling. Journal of Physics Condensed Matter, 2011, 23, 334210.	0.7	52
241	Formation of Bloch Flat Bands in Polar Twisted Bilayers without Magic Angles. Physical Review Letters, 2020, 124, 086401.	2.9	52
242	Large lattice-relaxation-induced electronic level shifts in randomCu1âˆ'xPdxalloys. Physical Review B, 1991, 44, 3387-3390.	1.1	51
243	Band gap of Hg chalcogenides: Symmetry-reduction-induced band-gap opening of materials with inverted band structures. Physical Review B, 2006, 74, .	1.1	51
244	Carrier-mediated long-range ferromagnetism in electron-doped Fe-C<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 Fe-N<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>incorporated graphene. Physical Review B, 2012, 86, .	1.1	50
245	High-throughput screening of chalcogenide single perovskites by first-principles calculations for photovoltaics. Journal Physics D: Applied Physics, 2018, 51, 474003.	1.3	50
246	First-principles study of the band gap tuning and doping control in CdSe_xTe_{1âˆ'x} alloy for high efficiency solar cell*. Chinese Physics B, 2019, 28, 086106.	0.7	50
247	Transmission electron microscopy investigation and first-principles calculation of the phase stability in epitaxial CuInS2 and CuGaSe2 films. Applied Physics Letters, 1999, 74, 2483-2485.	1.5	49
248	Origin of the significantly enhanced optical transitions in layered boron nitride. Physical Review B, 2012, 86, .	1.1	49
249	Origin of Novel Diffusions of Cu and Ag in Semiconductors: The Case of CdTe. Physical Review Letters, 2013, 110, 235901.	2.9	49
250	Chemical trends of defect formation in Si quantum dots: The case of group-III and group-V dopants. Physical Review B, 2007, 75, .	1.1	48
251	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
252	Ordering in semiconductor alloys. Applied Physics Letters, 1990, 56, 731-733.	1.5	47

#	Article	IF	Citations
253	Stability of theDXâˆ’Center in GaAs Quantum Dots. Physical Review Letters, 2005, 94, 185501.	2.9	47
254	Thermodynamically stable single-side hydrogenated graphene. Physical Review B, 2010, 82, .	1.1	47
255	Overcoming the Phase Inhomogeneity in Chemically Functionalized Graphene: The Case of Graphene Oxides. Physical Review Letters, 2013, 110, 085501.	2.9	47
256	Transition from Positive to Negative Photoconductance in Doped Hybrid Perovskite Semiconductors. Advanced Optical Materials, 2019, 7, 1900865.	3.6	47
257	Carrier-mediated stabilization of ferromagnetism in semiconductors: holes and electrons. Physica Status Solidi (B): Basic Research, 2006, 243, 2170-2187.	0.7	46
258	Theoretical and experimental studies of the ZnSe/CuInSe2heterojunction band offset. Applied Physics Letters, 1993, 62, 2557-2559.	1.5	45
259	Microstructure, optical property, and electronic band structure of cuprous oxide thin films. Journal of Applied Physics, 2011, 110, .	1.1	45
260	Electronic and magnetic properties of MnN versus MnAs. Applied Physics Letters, 2003, 82, 766-768.	1.5	44
261	First-principles study of roles of Cu and Cl in polycrystalline CdTe. Journal of Applied Physics, 2016, 119, .	1.1	44
262	Photocorrosion-Limited Maximum Efficiency of Solar Photoelectrochemical Water Splitting. Physical Review Applied, 2018, 10, .	1.5	44
263	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
264	Hexagonal boron nitride and 6H-SiC heterostructures. Applied Physics Letters, 2013, 102, .	1.5	43
265	Hydrogen Vibration Modes in GaP:N: The Pivotal Role of Nitrogen in Stabilizing theH2*Complex. Physical Review Letters, 2002, 88, 125506.	2.9	42
266	Prediction of the chemical trends of oxygen vacancy levels in binary metal oxides. Applied Physics Letters, 2011, 99, .	1.5	42
267	Absolute deformation potentials of Al, Si, and NaCl. Physical Review B, 1994, 50, 17797-17801.	1.1	41
268	Understanding Ultrahigh Doping: The Case of Boron in Silicon. Physical Review Letters, 2003, 90, 026103.	2.9	41
269	Magnetic states of zigzag graphene nanoribbons from first principles. Applied Physics Letters, 2009, 94, .	1.5	41
270	Exotic Geometrical and Electronic Properties in Hydrogenated Graphyne. Journal of Physical Chemistry C, 2013, 117, 11960-11967.	1.5	41

#	Article	IF	Citations
271	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
272	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
273	A novel viewpoint on the Cuî—¸Au phase diagram: The interplay between fixed ising energies and elastic effects. Acta Metallurgica, 1988, 36, 2239-2248.	2.1	40
274	Electronic Structure of â€œSequence Mutationsâ€•in OrderedGaInP2Alloys. Physical Review Letters, 1999, 83, 2010-2013.	2.9	40
275	Isoelectronic oxygen-related defect in CdTe crystals investigated using thermoelectric effect spectroscopy. Physical Review B, 2004, 69, .	1.1	40
276	Absence of volume metastability in bcc copper. Physical Review B, 1990, 41, 2699-2703.	1.1	39
277	Evolution of structural properties and formation of N-N split interstitials inGaAs1â˜'xNxalloys. Physical Review B, 2005, 71, .	1.1	39
278	Alignment of isovalent impurity levels: Oxygen impurity in II-VI semiconductors. Physical Review B, 2006, 73, .	1.1	39
279	Single-ion anisotropy, D-yaloshinskii-Moriya interaction, and negative magnetoresistance of the spin-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mfrac><mml:mrow><mml:mn>1</mml:mn></mml:mrow><mml:mrow><mml:mn>2</mml:mn></ xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>R</mml:mi><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></ Physical Review B, 2011, 83, .	1.1	39
280	Achieving High Volumetric Lithium Storage Capacity in Compact Carbon Materials with Controllable Nitrogen Doping. Advanced Functional Materials, 2019, 29, 1807441.	7.8	39
281	Thermodynamic Stability of(AlAs)n(GaAs)nSuperlattices and the RandomAl0.5Ga0.5AsAlloy. Physical Review Letters, 1988, 61, 1505-1508.	2.9	38
282	Theory of bonding charge density in Î²â€² NiAl. Acta Metallurgica Et Materialia, 1992, 40, 2155-2165.	1.9	38
283	Relativity-Induced Ordering and Phase Separation in Intermetallic Compounds. Europhysics Letters, 1993, 21, 221-226.	0.7	38
284	Effects of the wave function localization in AlInGaN quaternary alloys. Applied Physics Letters, 2007, 91, 061125.	1.5	38
285	Effect of hydrogen passivation on the electronic structure of ionic semiconductor nanostructures. Physical Review B, 2012, 85, .	1.1	38
286	Electronic origin of the conductivity imbalance between covalent and ionic amorphous semiconductors. Physical Review B, 2013, 87, .	1.1	38
287	The origin of electronic band structure anomaly in topological crystalline insulator group-IV tellurides. Npj Computational Materials, 2015, 1, .	3.5	38
288	Si₃AlP: A New Promising Material for Solar Cell Absorber. Journal of the American Chemical Society, 2012, 134, 12653-12657.	6.6	37

#	Article	IF	Citations
289	Optical anisotropy and spin polarization in ordered GaInP. Applied Physics Letters, 1994, 64, 1676-1678.	1.5	36
290	Origin of the doping bottleneck in semiconductor quantum dots: A first-principles study. Physical Review B, 2008, 77, .	1.1	36
291	First-Principles Study of Lithium Borocarbide as a Cathode Material for Rechargeable Li ion Batteries. Journal of Physical Chemistry Letters, 2011, 2, 1129-1132.	2.1	36
292	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
293	Atomic-scale understanding on the physics and control of intrinsic point defects in lead halide perovskites. Applied Physics Reviews, 2021, 8, .	5.5	36
294	Orderingâ€induced changes in the optical spectra of semiconductor alloys. Applied Physics Letters, 1988, 52, 311-313.	1.5	35
295	d-band excitations in II-VI semiconductors: A broken-symmetry approach to the core hole. Physical Review B, 1995, 52, 13975-13982.	1.1	35
296	Theory ofMnsupersaturation inSiandGe. Physical Review B, 2004, 70, .	1.1	35
297	Study of Phase Selectivity of Organicâ'Inorganic Hybrid Semiconductors. Chemistry of Materials, 2006, 18, 2805-2809.	3.2	35
298	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 mathvarian	1.1	35
299	Exceptional Optoelectronic Properties of Hydrogenated Bilayer Silicene. Physical Review X, 2014, 4, .	2.8	35
300	Identifying Optimal Inorganic Nanomaterials for Hybrid Solar Cells. Journal of Physical Chemistry C, 2009, 113, 18968-18972.	1.5	34
301	Negative spin-orbit bowing in semiconductor alloys. Physical Review B, 1989, 39, 6279-6282.	1.1	33
302	First-principles multiple-barrier diffusion theory: The case study of interstitial diffusion in CdTe. Physical Review B, 2015, 91, .	1.1	33
303	Inhomogeneous strain-induced half-metallicity in bent zigzag graphene nanoribbons. Npj Computational Materials, 2017, 3, .	3.5	33
304	Origin of the Stability and Transition from Anionic to Cationic Surface Ligand Passivation of All-Inorganic Cesium Lead Halide Perovskite Nanocrystals. Journal of Physical Chemistry Letters, 2020, 11, 652-658.	2.1	33
305	Hole-Mediated Stabilization of Cubic GaN. Physical Review Letters, 2004, 93, 216401.	2.9	32
306	Atomic structure of In2O3â€"ZnO systems. Applied Physics Letters, 2007, 90, 261904.	1.5	32

#	Article	IF	Citations
307	Symmetry of adsorption of oxygen at wurtzite AlN (0001) and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mo>(</mml:mo><mml:mn>000</mml:mn><mml:mover) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf	1.1	32
308	Origin of the Ising ferrimagnetism and spin-charge coupling in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>LuFe</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:ms Physical Review B, 2009, 80, .	1.1	32
309	First-principles study of electronic and diffusion properties of intrinsic defects in 4H-SiC. Journal of Applied Physics, 2020, 127, .	1.1	32
310	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
311	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
312	(111) oriented (GaAs)n(AlAs)nsuperlattices are direct bandâ€gap materials for allnâ€™s. Applied Physics Letters, 1988, 53, 2077-2079.	1.5	30
313	Effects of ordering on the electron effective mass and strain deformation potential inGaInP2: Deficiencies of thekâ‹…pmodel. Physical Review B, 1995, 52, 13992-13997.	1.1	30
314	Origin of the Bismuth-Induced Decohesion of Nickel and Copper Grain Boundaries. Physical Review Letters, 2013, 111, 055502.	2.9	30
315	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
316	Realistic dimension-independent approach for charged-defect calculations in semiconductors. Physical Review B, 2020, 101, .	1.1	30
317	Local structure ofCuIn3Se5:X-ray absorption fine structure study and first-principles calculations. Physical Review B, 2003, 68, .	1.1	29
318	Atomistic origins of the phase transition mechanism in Ge2Sb2Te5. Journal of Applied Physics, 2009, 106, .	1.1	29
319	Persistent Medium-Range Order and Anomalous Liquid Properties ofAl1â^'xCuxAlloys. Physical Review Letters, 2012, 108, 115901.	2.9	29
320	Effects of deposition termination on Cu2ZnSnSe4 device characteristics. Thin Solid Films, 2015, 582, 184-187.	0.8	29
321	Design of shallow acceptors in ZnO through compensated donor-acceptor complexes: A density functional calculation. Physical Review B, 2009, 80, .	1.1	28
322	Origin of the diverse behavior of oxygen vacancies inABO3perovskites: A symmetry based analysis. Physical Review B, 2012, 85, .	1.1	28
323	Origin of Efficiency Enhancement by Lattice Expansion in Hybrid-Perovskite Solar Cells. Physical Review Letters, 2022, 128, 136401.	2.9	28
324	Strain effects on the spectra of spontaneously ordered GaxIn1â^'xP. Applied Physics Letters, 1994, 64, 757-759.	1.5	27

#	Article	IF	Citations
325	Unintentional doping and compensation effects of carbon in metal-organic chemical-vapor deposition fabricated ZnO thin films. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2006, 24, 1213-1217.	0.9	27
326	Ferrimagnetic Fe-doped GaN: An unusual magnetic phase in dilute magnetic semiconductors. Physical Review B, 2009, 79, .	1.1	27
327	Theoretical investigation of atomic and electronic structures of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Ga</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub> Physical Review B, 2009, 80, .	1.1	27
328	Controlling doping in graphene through a SiC substrate: A first-principles study. Physical Review B, 2011, 83, .	1.1	27
329	Possible effects of oxygen in Te-rich Î£3 (112) grain boundaries in CdTe. Solid State Communications, 2012, 152, 1744-1747.	0.9	27
330	Electronic structure ofM3ISb-type filled tetrahedral semiconductors. Physical Review B, 1987, 35, 3952-3961.	1.1	26
331	Point-charge electrostatics in disordered alloys. Physical Review B, 1996, 54, 7843-7856.	1.1	26
332	Design of shallow acceptors in ZnO through early transition metals codoped with N acceptors. Physical Review B, 2011, 83, .	1.1	26
333	Effect of surface passivation on dopant distribution in Si quantum dots: The case of B and P doping. Applied Physics Letters, 2011, 98, .	1.5	26
334	Phosphorus Diffusion Mechanisms and Deep Incorporation in Polycrystalline and Single-Crystalline CdTe. Physical Review Applied, 2016, 5, .	1.5	26
335	Electronic structure of IIâ€“VI compounds and their alloys â€” role of cation d bands. Journal of Crystal Growth, 1988, 86, 1-7.	0.7	25
336	Structural and electronic properties ofZnGeAs2. Physical Review B, 2001, 63, .	1.1	25
337	Atomically Abrupt Liquid-Oxide Interface Stabilized by Self-Regulated Interfacial Defects: The Case of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Al</mml:mi><mml:mo>/</mml:mo><mml:msub><mml:mi>Al</mml:mi><mml:mn>2</mml:mn></mml:msub> mathvariant="bold">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>Interfaces. Physical Review Letters, 2012, 108, 226105.	2.9	25
338	Origin of the Distinct Diffusion Behaviors of Cu and Ag in Covalent and Ionic Semiconductors. Physical Review Letters, 2016, 117, 165901.	2.9	25
339	The Coulomb interaction in van der Waals heterostructures. Science China: Physics, Mechanics and Astronomy, 2019, 62, 1.	2.0	25
340	Prediction and observation of IIâ€“VI/CuInSe2 heterojunction band offsets. Journal of Electron Spectroscopy and Related Phenomena, 1994, 68, 185-193.	0.8	24
341	Opening space for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>H</mml:mtext><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:ma Cointercalation of graphite with lithium and small organic molecules. Physical Review B, 2008, 78, .	1.1	24
342	Origin of the Diverse Melting Behaviors of Intermediate-Size Nanoclusters: Theoretical Study of AlN(N= 51â^’58, 64). Journal of the American Chemical Society, 2010, 132, 18287-18291.	6.6	24

#	Article	IF	Citations
343	Passivation of deep electronic states of partial dislocations in GaAs: A theoretical study. Applied Physics Letters, 2010, 96, .	1.5	24
344	First-principles study of defect properties of zinc blende MgTe. Physical Review B, 2011, 83, .	1.1	24
345	Correlation between the electronic structures and diffusion paths of interstitial defects in semiconductors: The case of CdTe. Physical Review B, 2014, 90, .	1.1	24
346	Revisit of the band gaps of rutile SnO₂ and TiO₂: a first-principles study. Journal of Semiconductors, 2019, 40, 092101.	2.0	24
347	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:msub><mml: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
348	Donorâ€“donor binding in semiconductors: Engineering shallow donor levels for ZnTe. Applied Physics Letters, 2003, 83, 3522-3524.	1.5	23
349	First-principles study of Mn-induced local magnetic moments in host semiconductors. Physical Review B, 2005, 71, .	1.1	23
350	Probing deactivations in Nitrogen doped ZnO by vibrational signatures: A first principles study. Physica B: Condensed Matter, 2006, 376-377, 686-689.	1.3	23
351	Electron-mediated ferromagnetism and negativesâ^'dexchange splitting in semiconductors. Physical Review B, 2006, 73, .	1.1	23
352	Comparative study of defect transition energy calculation methods: The case of oxygen vacancy in In<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>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>and ZnO. Physical Review B, 2012, 86, .	1.1	23
353	H-stabilized shallow acceptors in N-doped ZnO. Physical Review B, 2015, 92, .	1.1	23
354	Suppress carrier recombination by introducing defects: The case of Si solar cell. Applied Physics Letters, 2016, 108, .	1.5	23
355	Comment on â€˜â€˜Origins of compositional order in NiPt alloysâ€™â€™. Physical Review Letters, 1992, 68, 1961-1961.	2.9	22
356	Crystal structure and defect reactions in the kesterite solar cell absorber Cu[sub 2]ZnSnS[sub 4] (CZTS): Theoretical insights. , 2011, , .		22
357	Carrier providers or killers: The case of Cu defects in CdTe. Applied Physics Letters, 2017, 111, 042106.	1.5	22
358	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
359	Nanowire Quantum Dot Surface Engineering for High Temperature Single Photon Emission. ACS Nano, 2019, 13, 13492-13500.	7.3	22
360	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

#	Article	IF	Citations
361	Shape Control of Al Nanoclusters by Ligand Size. Journal of the American Chemical Society, 2009, 131, 8522-8526.	6.6	21
362	Tuning doping site and type by strain: Enhanced -type doping in Li doped ZnO. Solid State Communications, 2011, 151, 1437-1439.	0.9	21
363	Defect properties of Sb- and Bi-doped CuInSe2: The effect of the deep lone-pair s states. Applied Physics Letters, 2014, 105, .	1.5	21
364	Chemical trends of stability and band alignment of lattice-matched II-VI/III-V semiconductor interfaces. Physical Review B, 2015, 91, .	1.1	21
365	Calculation of the valence band offsets of common-anion semiconductor heterojunctions from core levels: The role of cation d orbitals. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 1987, 5, 1239.	1.6	20
366	Chemical trends in band offsets of Zn- and Mn-based II-VI superlattices:d-level pinning and offset compression. Physical Review B, 1996, 53, R10457-R10460.	1.1	20
367	Bond-length distribution in tetrahedral versus octahedral semiconductor alloys: The case ofGa1â^'xInxN. Physical Review B, 1997, 56, 13872-13877.	1.1	20
368	Mutual Passivation of Donors and Isovalent Nitrogen in GaAs. Physical Review Letters, 2006, 96, 035505.	2.9	20
369	Impurity-induced phase stabilization of semiconductors. Applied Physics Letters, 2006, 89, 011907.	1.5	20
370	Theoretical study of stability and electronic structure of Li(Mg,Zn)N alloys: A candidate for solid state lighting. Physical Review B, 2007, 76, .	1.1	20
371	Structural and electronic properties of [0001] AlN nanowires: A first-principles study. Journal of Applied Physics, 2008, 104, 084313.	1.1	20
372	Understanding the Clean Interface between Covalent Si and Ionic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Al</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2009, 103, 116101.	2.9	20
373	Symmetry-breaking-induced enhancement of visible light absorption in delafossite alloys. Applied Physics Letters, 2009, 94, 251907.	1.5	20
374	Ordering-enhanced dislocation glide in III-V alloys. Journal of Applied Physics, 2013, 114, .	1.1	20
375	Ordering-induced direct-to-indirect band gap transition in multication semiconductor compounds. Physical Review B, 2015, 91, .	1.1	20
376	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
377	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
378	Microscopic Theory of Hysteretic Hydrogen Adsorption in Nanoporous Materials. Journal of the American Chemical Society, 2010, 132, 1510-1511.	6.6	19

#	Article	IF	Citations
379	P-type doping of lithium peroxide with carbon sheets. Applied Physics Letters, 2012, 101, .	1.5	19
380	Origin of polymorphism of the two-dimensional group-IV monochalcogenides. Physical Review B, 2017, 96, .	1.1	19
381	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
382	Ground state structures of intermetallic compounds: A first-principles Ising model. Solid State Communications, 1991, 78, 583-588.	0.9	18
383	Transition from ferromagnetism to antiferromagnetism in Ga1â^'xMnxN. Journal of Applied Physics, 2005, 98, 083905.	1.1	18
384	Origin of the phase transition of AlN, GaN, and ZnO nanowires. Applied Physics Letters, 2009, 94, .	1.5	18
385	Enhancing dopant solubility via epitaxial surfactant growth. Physical Review B, 2009, 80, .	1.1	18
386	Charge-driven structural transformation and valence versatility of boron sheets in magnesium borides. Physical Review B, 2011, 83, .	1.1	18
387	Bowing of the defect formation energy in semiconductor alloys. Physical Review B, 2013, 87, .	1.1	18
388	First-principles phase diagrams of pseudoternary chalcopyriteâ€“zinc-blende alloys. Physical Review B, 1993, 47, 9985-9988.	1.1	17
389	E1,E2, andE0â€²transitions and pressure dependence in orderedGa0.5In0.5P. Physical Review B, 1995, 51, 13097-13102.	1.1	17
390	Computational design of a material for high-efficiency spin-polarized electron source. Applied Physics Letters, 2002, 81, 3957-3959.	1.5	17
391	Origin of Bonding between the SWCNT and the Fe₃O₄(001) Surface and the Enhanced Electrical Conductivity. Journal of Physical Chemistry Letters, 2011, 2, 2853-2858.	2.1	17
392	Prediction of (TiO₂)_x(Cu₂O)_yalloys for efficient photoelectrochemical water splitting. Physical Chemistry Chemical Physics, 2013, 15, 1778-1781.	1.3	17
393	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:mo>(</mml:mo><mml:mi>M</mml:mi><mml:mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mrow><mml:mo>(</mml:mo><mml:mi>M</mml:mi><mml:mi>Physical Review B, 2015, 92, .	2.1	17
394	Microscopic mechanism of the tunable band gap in potassium-doped few-layer black phosphorus. Physical Review B, 2017, 96, .	1.1	17
395	Band structure engineering and defect control of oxides for energy applications. Chinese Physics B, 2018, 27, 117104.	0.7	17
396	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

#	Article	IF	Citations
397	First-principles study of defect control in thin-film solar cell materials. Science China: Physics, Mechanics and Astronomy, 2021, 64, 1.	2.0	17
398	Steps on As-Terminated Ge(001) Revisited: Theory versus Experiment. Physical Review Letters, 2001, 87, 166104.	2.9	16
399	Exploring Emerging Photovoltaic Materials Beyond Perovskite: The Case of Skutterudite. Chemistry of Materials, 2017, 29, 9429-9435.	3.2	16
400	Chemical Design of Direct-Gap Light-Emitting Silicon. Physical Review Letters, 2002, 89, 076802.	2.9	15
401	Mg acceptor energy levels in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Al</mml:mi><mml:mi>x</mml:mi></mml:msub><mml:msub><mml:mi mathvariant="normal">In</mml:mi><mml:mi>y</mml:mi></mml:msub><mml:msub><mml:mi mathvariant="normal">Ga</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi><mml:mo>â^’</mml:mo><mml:mi>y</mml:mi></mml:mrow></mml:msub><mml:msub><mml:mi mathvariant="normal">N</mml:mi></mml:msub></mml:mrow></mml:math> quaternar. Physical Review B, 2008, 77, .	1.1	15
402	Electronic and optical properties of CoX2O4 (Xâ€‰=â€‰Al, Ga, In) alloys. Applied Physics Letters, 2012, 100, .	1.5	15
403	Pathways toward higher performance CdS/CdTe devices: Te exposure of CdTe surface before ZnTe:Cu/Ti contacting. Thin Solid Films, 2013, 535, 237-240.	0.8	15
404	Air Passivation of Chalcogen Vacancies in Twoâ€Đimensional Semiconductors. Angewandte Chemie, 2016, 128, 977-980.	1.6	15
405	Strong Coupled Magnetic and Electric Ordering in Monolayer of Metal Thio(seleno)phosphates. Chinese Physics Letters, 2021, 38, 077501.	1.3	15
406	Theoretical investigation of halide perovskites for solar cell and optoelectronic applications*. Chinese Physics B, 2020, 29, 108401.	0.7	15
407	Effects of covalency,pâ^’dcoupling, and epitaxial strain on the band offsets of II-VI semiconductors. Physical Review B, 2003, 68, .	1.1	14
408	Photoinduced cation interstitial diffusion in IIâ€“VI semiconductors. Physical Review B, 2005, 72, .	1.1	14
409	Exchange-induced negative-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>U</mml:mi></mml:math>charge order in N-doped<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>WO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> A spin Peierls-like system. Physical Review B, 2009, 80, .	1.1	14
410	Quaternary semiconductors with positive crystal field splitting: Potential high-efficiency spin-polarized electron sources. Applied Physics Letters, 2009, 95, .	1.5	14
411	Origin of Enhanced Dihydrogen-Metal Interaction in Carboxylate Bridged<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Cu</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>â€“Paddle-Wheel Frameworks. Physical Review Letters, 2010, 105, 236105.	2.9	14
412	First-Principles Study of Electronic Structure and Hydrogen Adsorption of 3d Transition Metal Exposed Paddle Wheel Frameworks. Journal of Physical Chemistry C, 2012, 116, 7386-7392.	1.5	14
413	Type-IIâ†’type-I transition in (GaX)n/(InX)n(001) superlattices (X=P, Sb) as a function of periodn. Physical Review B, 1994, 50, 8094-8097.	1.1	13
414	Step Structures on III-V Phosphide (001) Surfaces: How Do Steps and Sb affect CuPt Ordering ofGaInP2?. Physical Review Letters, 2005, 94, 096101.	2.9	13

#	Article	IF	Citations
415	Relaxation models of the (110) zinc-blende III-V semiconductor surfaces: Density functional study. Physical Review B, 2008, 78, .	1.1	13
416	Origin of the failed ensemble average rule for the band gaps of disordered nonisovalent semiconductor alloys. Physical Review B, 2014, 90, .	1.1	13
417	Monitoring the stability of organometallic perovskite thin films. Journal of Materials Chemistry A, 2015, 3, 21940-21945.	5.2	13
418	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
419	Mechanism of Synergistic Effects of Neutron- and Gamma-Ray-Radiated PNP Bipolar Transistors. ACS Applied Electronic Materials, 2019, 1, 538-547.	2.0	13
420	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
421	Stability of a planar-defect structure of the wurtzite AlN<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mrow><mml:mo>(</mml:mo><mml:mrow><mml:mn>10</mml:mn><mml:mover) Tj ETQq1 1 0.784	1.1	12
422	Density functional study. Physical Review B, 2009, 80, . Effects of Side-Chain and Electron Exchange Correlation on the Band Structure of Perylene Diimide Liquid Crystals: A Density Functional Study. Journal of Physical Chemistry B, 2009, 113, 5376-5380.	1.2	12
423	Period-doubling reconstructions of semiconductor partial dislocations. NPG Asia Materials, 2015, 7, e216-e216.	3.8	12
424	First-principles calculation of the formation energies of ordered and disordered phases of AlAs-GaAs. Physical Review B, 1989, 40, 1642-1646.	1.1	11
425	Point-ion versus density functional calculations of electric field gradients in ordered GaInP2. Journal of Chemical Physics, 1997, 107, 1931-1935.	1.2	11
426	The roles of CU impurity states in CdTe thin film solar cells. , 2010, , .		11
427	Unusual nonlinear strain dependence of valence-band splitting in ZnO. Physical Review B, 2012, 86, .	1.1	11
428	Wild band edges: The role of bandgap grading and band-edge fluctuations in high-efficiency chalcogenide devices. , 2016, , .		11
429	Antimony Diffusion in CdTe. IEEE Journal of Photovoltaics, 2017, 7, 870-873.	1.5	11
430	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> with Group-V Elements: A First-Principles Study. Physical Review Applied, 2021, 15, .	1.5	11
431	Ground-state structure of coherent lattice-mismatched zinc-blendeA1â^'xBxCsemiconductor alloys (x=0.25and 0.75). Physical Review B, 2008, 77, .	1.1	10
432	First-principles study of iron segregation into silicon â^5 grain boundary. Journal of Applied Physics, 2010, 107, 093713.	1.1	10

#	Article	IF	Citations
433	Overcoming doping bottleneck by using surfactant and strain. Frontiers of Materials Science, 2011, 5, 335-341.	1.1	10
434	Selection rule of preferred doping site for n-type oxides. Applied Physics Letters, 2012, 100, 262109.	1.5	10
435	Chemical trends of magnetic interaction in Mn-doped III-V semiconductors. Applied Physics Letters, 2013, 102, 122409.	1.5	10
436	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
437	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
438	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
439	Origin of High- T_C Ferromagnetism in Isovalent-Doped III-V Semiconductors. Physical Review Applied, 2019, 11, .	1.5	10
440	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
441	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
442	Origin of Irradiation Synergistic Effects in Silicon Bipolar Transistors. ACS Applied Electronic Materials, 2020, 2, 3783-3793.	2.0	10
443	Design of Multifunctional Quinternary Metal-Halide Perovskite Compounds Based on Cationâ€“Anion Co-Ordering. Chemistry of Materials, 2020, 32, 5949-5957.	3.2	10
444	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
445	General Model for Defect Dynamics in Ionizingâ€Irradiated SiO₂â€Si Structures. Small, 2022, 18, e2107516.	5.2	10
446	Comment on "Coulomb Energy in Pseudobinary Alloys". Physical Review Letters, 1987, 59, 2613-2613.	2.9	9
447	Common-anion rule and its limits: Photoemission studies ofCuInxGa1â^'xSe2-Ge andCuxAg1â^'xInSe2-Ge interfaces. Physical Review B, 1987, 36, 9388-9391.	1.1	9
448	Chen, Gong, and Wei Reply:. Physical Review Letters, 2007, 99, .	2.9	9
449	Effect of intermixing at CdS/CdTe interface on defect properties. Applied Physics Letters, 2016, 109, 042105.	1.5	9
450	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

#	Article	IF	Citations
451	Origin of anomalous band-gap bowing in two-dimensional tin-lead mixed perovskite alloys. Physical Review B, 2021, 104, .	1.1	9
452	Perspective on the band structure engineering and doping control of transparent conducting materials. Applied Physics Letters, 2021, 119, .	1.5	9
453	Universal Theory and Basic Rules of Strain-Dependent Doping Behaviors in Semiconductors. Chinese Physics Letters, 2021, 38, 087103.	1.3	9
454	Theory of reflectance-difference spectroscopy in ordered III-V semiconductor alloys. Physical Review B, 1995, 51, 14110-14114.	1.1	8
455	Nitrogen solubility and N-induced defect complexes in epitaxial GaAs:N. Physica B: Condensed Matter, 2001, 308-310, 839-842.	1.3	8
456	Growth Model for Atomic Ordering: The Case for Quadruple-Period Ordering in GaAsSb Alloys. Physical Review Letters, 2003, 90, 026102.	2.9	8
457	Carrier-induced enhancement and suppression of ferromagnetism in Zn_{1-x}Cr_xTe and Ga_{1-x}Cr_xAs: origin of the spinodal decomposition. New Journal of Physics, 2008, 10, 113007.	1.2	8
458	Comment on â€œMechanisms of Postsynthesis Doping of Boron Nitride Nanostructures with Carbon from First-Principles Simulationsâ€• Physical Review Letters, 2011, 107, 239601; discussion 239602.	2.9	8
459	Polymerization of defect states at dislocation cores in InAs. Journal of Applied Physics, 2016, 119, 045706.	1.1	8
460	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
461	Decoupling of the Electrical and Thermal Transports in Strongly Coupled Interlayer Materials. Journal of Physical Chemistry Letters, 2021, 12, 7832-7839.	2.1	8
462	Clarification of the relative magnitude of exciton binding energies in ZnO and SnO2. Applied Physics Letters, 2022, 120, .	1.5	8
463	Stability of atomic and diatomic hydrogen in fcc palladium. Solid State Communications, 1990, 73, 327-330.	0.9	7
464	Effects of alloying, ordering, and strain on the exchange parameters of II-VI dilute magnetic semiconductors. Physical Review B, 2004, 70, .	1.1	7
465	Walsh, Da Silva, and Wei Reply:. Physical Review Letters, 2009, 102, .	2.9	7
466	Design of quaternary chalcogenide photovoltaic absorbers through cation mutation. , 2009, , .		7
467	Overcoming Bipolar Doping Difficulty in Wide Gap Semiconductors. , 2011, , 213-239.		7
468	Creating intermediate bands in ZnTe via co-alloying approach. Applied Physics Express, 2014, 7, 121201.	1.1	7

#	Article	IF	Citations
469	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
470	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:mi><mml:mn>2</mml:mn></mml 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
471	Band gap anomaly in cuprous halides. Computational Materials Science, 2022, 203, 111157.	1.4	7
472	Temperature effect on charge-state transition levels of defects in semiconductors. Physical Review B, 2022, 105, .	1.1	7
473	Elements of doping engineering in semiconductors. , 1999, , .		6
474	Band coupling model of electron and hole mediated ferromagnetism in semiconductors: the case of GaN. , 2008, , .		6
475	Origin of charge separation in III-nitride nanowires under strain. Applied Physics Letters, 2011, 99, 262103.	1.5	6
476	Strong asymmetrical doping properties of spinel CoAl2O4. Journal of Applied Physics, 2012, 111, 093723.	1.1	6
477	Origin of anomalous strain effects on the molecular adsorption on boron-doped graphene. Journal of Chemical Physics, 2013, 139, 044709.	1.2	6
478	O-O bonding stabilized zinc vacancy as origin of p-type doping on Î£7 ZnO grain boundary. Journal of Applied Physics, 2015, 118, 045708.	1.1	6
479	Stable interface structures of heterovalent semiconductor superlattices: The case of (GaSb) (ZnTe). Computational Materials Science, 2015, 98, 340-344.	1.4	6
480	Magnetic origin of phase stability in cubic Î³-MoN. Applied Physics Letters, 2018, 113, 221901.	1.5	6
481	Atomic-Ordering-Induced Quantum Phase Transition between Topological Crystalline Insulator and Z 2 Topological Insulator. Chinese Physics Letters, 2018, 35, 057301.	1.3	6
482	Self-Catalyzed Sensitization of CuO Nanowires via a Solvent-free Click Reaction. Langmuir, 2020, 36, 14539-14545.	1.6	6
483	Strain induced spin-splitting and half-metallicity in antiferromagnetic bilayer silicene under bending. Physical Chemistry Chemical Physics, 2020, 22, 11567-11571.	1.3	6
484	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		

#	Article	IF	Citations
487	Electronic Structure and Stability of Spinel Oxides. Japanese Journal of Applied Physics, 2000, 39, 251.	0.8	5
488	Long and Short Range Ordering of CuInSe₂. Japanese Journal of Applied Physics, 2000, 39, 411.	0.8	5
489	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
490	Structural, Electronic and Defect Properties of Cu2ZnSn(S,Se)4 Alloys. Materials Research Society Symposia Proceedings, 2011, 1370, 55.	0.1	5
491	Control of one-dimensional magnetism in graphene via spontaneous hydrogenation of the grain boundary. Physical Chemistry Chemical Physics, 2013, 15, 8271.	1.3	5
492	Chemical trend of the formation energies of the group-III and group-V dopants in Si quantum dots. Physical Review B, 2013, 87, .	1.1	5
493	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
494	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
495	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
496	Carrier-stabilized hexagonal Ge. Physical Review B, 2021, 103, .	1.1	5
497	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
498	Effects of co-doping in semiconductors: CdTe. Physical Review B, 2021, 104, .	1.1	5
499	Effects of N on the electronic structures of H defects in IIIâ€“V semiconductors. Optical Materials, 2004, 25, 261-269.	1.7	4
500	Ordering induced direct and indirect transitions in semiconductor alloys. Physical Review B, 2006, 74, .	1.1	4
501	The Mechanism of J-V â€œRoll-Overâ€•in CdS/CdTe Devices. Materials Research Society Symposia Proceedings, 2007, 1012, 1.	0.1	4
502	Delafossite-alloy photoelectrodes for PEC hydrogen production: a density functional theory study. Proceedings of SPIE, 2010, , .	0.8	4
503	Kesterite successes, ongoing work, and challenges: A perspective from vacuum deposition. , 2012, , .		4
504	Stability and electronic structures of Cu<inf>x</inf>S solar cell absorbers. , 2012, , .		4

#	Article	IF	Citations
505	Tunable Anderson Localization in Hydrogenated Graphene Based on the Electric Field Effect. Physical Review Letters, 2013, 111, 216801.	2.9	4
506	Enhancing structural transition by carrier and quantum confinement: Stabilization of cubic InN quantum dots by Mn incorporation. Applied Physics Letters, 2013, 103, .	1.5	4
507	Designing Dirac semimetals with a honeycomb Na₃Bi-lattice via isovalent cation substitution. Journal of Materials Chemistry C, 2020, 8, 1257-1264.	2.7	4
508	Unconventional deformation potential and half-metallicity in zigzag nanoribbons of 2D-Xenes. Physical Chemistry Chemical Physics, 2020, 22, 7294-7299.	1.3	4
509	Enhancing magnetic dipole emission in Eu-doped <mml:math 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 ETQq1 1 0.784314 rgBT /Ov	1.1	4
510	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
511	Instability of diatomic deuterium in fcc palladium. Journal of Fusion Energy, 1990, 9, 367-370.	0.5	3
512	Prediction of New Fingerprints of Ordering in GaInP₂ Alloys. Materials Research Society Symposia Proceedings, 1995, 417, 103.	0.1	3
513	Revisiting the defect physics in CuInSe/sub 2/ and CuGaSe/sub 2/. , 0, , .		3
514	Synthesis and Characterization of Nitrogen-Doped ZnO Films Grown by MOCVD. , 2006, , 43-83.		3
515	Ordered ground state wurtzite alloys from zinc-blende parent compounds. Physical Review B, 2009, 80, .	1.1	3
516	Spatial charge distribution and conductivities of the LaAlO3/SrTiO3 interfaces: A theoretical study. Solid State Communications, 2011, 151, 21-23.	0.9	3
517	Electron-limiting defect complex in hyperdoped GaAs: TheDDXcenter. Physical Review B, 2013, 87, .	1.1	3
518	XiangetÂal.Reply:. Physical Review Letters, 2014, 112, 199802.	2.9	3
519	Metal compound semiconductors functionalized by polymers and their photosensitive properties. Applied Physics Reviews, 2016, 3, .	5.5	3
520	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
521	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
522	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:mi mathvariant="normal">S</mml:mi></mml:mrow><mml:mrow><mml:mi>y</mml:mi></mml:msub><mml:msub><mml:mi>Se</mml:mi> Physical Review Applied, 2020, 13, .	4.3	3

#	Article	IF	Citations
523	Origin of hydrogen passivation in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>4</mml:mn><mml:mi>H</mml:mi><mml:mo></mml:mo><mml:mrow></mml:mrow></mml:mrow></mml:math> -SiC. Physical Review Materials, 2021, 5, .	0.9	3
524	Application of generalized Bloch method: Strain engineering of low dimensional materials through inhomogeneous strains. Chinese Science Bulletin, 2021, 66, 674-684.	0.4	3
525	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
526	Structure Investigations of Several In-rich (Cu₂Se)_x(In₂Se₃)_{1â^'x} Compositions: From Local Structure to Long Range Order. Materials Research Society Symposia Proceedings, 2001, 668, 1.	0.1	2
527	Effects of Ordering on Physical Properties of Semiconductor Alloys. , 2002, , 423-450.		2
528	Effect ofZnon the cation vacancyâ€“isoelectronic oxygen pair inCd1â^'xZnxTecrystals. Physical Review B, 2004, 70, .	1.1	2
529	Impurity-stabilized zinc-blende phase of wurtzite compounds. Journal of Physics and Chemistry of Solids, 2005, 66, 2008-2010.	1.9	2
530	Local charge neutgrality condition, Fermi level, and carrier compensation of CdTe polycrystalline thin film in CdS/CdTe solar cells. , 2010, , .		2
531	Carrier density and compensation in semiconductors with multi dopants and multi transition energy levels: The case of Cu impurity in CdTe. , 2011, , .		2
532	Strain effect on the diffusion of interstitial Mn in GaAs. Journal of Physics Condensed Matter, 2012, 24, 215801.	0.7	2
533	Magnetic property of transition metal-Si atomic line on silicon Î£3 grain boundary: A theoretical study. Journal of Applied Physics, 2014, 115, 223906.	1.1	2
534	Origin of the structural diversity of M2O3 (M = Al, Ga, In). Computational Materials Science, 2015, 104, 35-39.	1.4	2
535	Nonisovalent Si-III-V and Si-II-VI alloys: Covalent, ionic, and mixed phases. Physical Review B, 2017, 96, .	1.1	2
536	Preface for Special Topic: Earth abundant materials in solar cells. APL Materials, 2018, 6, .	2.2	2
537	Chemical trend of a Cu impurity in Zn chalcogenides. Physical Review B, 2020, 101, .	1.1	2
538	Chemical trends of cation-vacancy-induced d⁰ ferromagnetism in dilute zinc chalcogenides. Journal Physics D: Applied Physics, 2021, 54, 375001.	1.3	2
539	Functionalizing Two-Dimensional Materials for Energy Applications. , 2020, , 567-603.		2
540	Band Structure and Stability of Ternary Semiconductor Polytypes. Japanese Journal of Applied Physics, 2000, 39, 237.	0.8	2

#	Article	IF	Citations
541	Dependence of Optical Properties of Semiconductor Alloys on Long Range Order, Strain and Pressure. Materials Research Society Symposia Proceedings, 1995, 417, 3.	0.1	1
542	Electronic structure and doping of p-type transparent conducting oxides. , 0, , .		1
543	Epitaxially stabilized AgGaSe2 for high-efficiency spin-polarized electron source. Journal of Physics and Chemistry of Solids, 2003, 64, 1881-1885.	1.9	1
544	Filling the green gap: A firstâ€principles study of the LiMg_{1â€x}Zn_xN alloy. Physica Status Solidi C: Current Topics in Solid State Physics, 2008, 5, 2326-2328.	0.8	1
545	Comparison of atomistic simulations and statistical theories for variable degree of long-range order in semiconductor alloys. Physical Review B, 2009, 80, .	1.1	1
546	Role of d Orbitals in Valence-Band Offsets of Common-Anion Semiconductors. Perspectives in Condensed Matter Physics, 1988, , 200-203.	0.1	1
547	Local Structure Around Te in Heavily Doped GaAs:Te using X-Ray Absorption Fine Structure. Acta Physica Polonica A, 2012, 121, 879-882.	0.2	1
548	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
549	Band Structure and Electronic Excitations in Cdl-xMnxTe. Materials Research Society Symposia Proceedings, 1986, 89, 197.	0.1	0
550	Work in the solid state theory group at the solar energy research institute. Solar Cells, 1987, 21, 458-459.	0.6	0
551	ELECTRONIC STRUCTURE OF II-VI SEMICONDUCTORS AND THEIR ALLOYS. , 1993, , 71-101.		0
552	Structural instability in zinc-blende semiconductors. Ferroelectrics, 1994, 155, 127-132.	0.3	0
553	Spin polarization of photoelectrons from ordered semiconductor alloys. , 1998, , .		0
554	Nitrogen-Stabilized H2* Defects in GaP:N. Materials Research Society Symposia Proceedings, 2002, 719, 631.	0.1	0
555	Quadruple-period ordering in MBE GaAsSb alloys. Materials Research Society Symposia Proceedings, 2003, 794, 49.	0.1	0
556	Electronic and optical properties ofÎ´-layerGaN/(GaAs)nsuperlattices. Physical Review B, 2003, 67, .	1.1	0
557	Design of shallow p-type dopants in ZnO. Conference Record of the IEEE Photovoltaic Specialists Conference, 2008, , .	0.0	0
558	Structural, electronic, and optical properties of the In<inf>2</inf>O<inf>3</inf>(ZnO)<inf>n</inf> system. , 2009, , .		0

#	Article	IF	Citations
559	Graphene Adsorbed on Corundum Surface: Clean Interface and Band Gap Opening. Materials Research Society Symposia Proceedings, 2012, 1407, 131.	0.1	0
560	Rational design of semiconductors for photoelectrochemical water splitting. , 2013, , .		0
561	Kesterite successes, ongoing work, and challenges: A perspective from vacuum deposition. , 2013, , .		0
562	First-principles Study of Defect Control in Solar Cell Materials. , 2015, , .		0
563	Notice of Removal Antimony diffusion in CdTe. , 2017, , .		0
564	Functionalizing Two-Dimensional Materials for Energy Applications. , 2018, , 1-37.		0
565	Hole-Induced Spontaneous Mutual Annihilation of Dislocation Pairs. Journal of Physical Chemistry Letters, 2019, 10, 7421-7425.	2.1	0
566	Group velocity matters for accurate prediction of phonon-limited carrier mobility*. Chinese Physics B, 2021, 30, 087201.	0.7	0
567	Large-Scale Ab Initio Study of Size, Shape, and Doping Effects on Electronic Structure of Nanocrystals. , 2009, , 193-211.		0
568	Ab-initio assessment of new sulfo-iodide compounds as candidate top-cell materials for silicon-based multi-junction tandem solar cells. , 2019, , .		0
569	Accurate and effective computation of the multi-phonon nonradiative transition. Science China: Physics, Mechanics and Astronomy, 2020, 63, 1.	2.0	0
570	Phase transition behavior of heterostructural alloys: Effects of size mismatch and site preference. Physical Review B, 2022, 105, .	1.1	0