Su-Huai Wei

List of Publications by Citations

546 papers	47,616 citations	113 h-index	203 g-index
578 ext. papers	52,213 ext. citations	5.3 avg, IF	7.84 L-index

#	Paper	IF	Citations
546	Special quasirandom structures. *Physical Review Letters*, **1990**, 65, 353-356	7.4	2054
545	Stabilizing Perovskite Structures by Tuning Tolerance Factor: Formation of Formamidinium and Cesium Lead Iodide Solid-State Alloys. *Chemistry of Materials*, **2016**, 28, 284-292	9.6	1186
544	Defect physics of the CuInSe2 chalcopyrite semiconductor. *Physical Review B*, **1998**, 57, 9642-9656	3.3	1128
543	Origin of p-type doping difficulty in ZnO: The impurity perspective. *Physical Review B*, **2002**, 66,	3.3	998
542	Classification of lattice defects in the kesterite Cu2ZnSnS4 and Cu2ZnSnSe4 earth-abundant solar cell absorbers. *Advanced Materials*, **2013**, 25, 1522-39	24	979
541	Halide perovskite materials for solar cells: a theoretical review. *Journal of Materials Chemistry A*, **2015**, 3, 8926-8942	13	882
540	Electronic properties of random alloys: Special quasirandom structures. *Physical Review B*, **1990**, 42, 9622-9649	3.3	688
539	Design of narrow-gap TiO2: a passivated codoping approach for enhanced photoelectrochemical activity. *Physical Review Letters*, **2009**, 102, 036402	7.4	661
538	Calculated natural band offsets of all II–VI and III–V semiconductors: Chemical trends and the role of cation d orbitals. *Applied Physics Letters*, **1998**, 72, 2011-2013	3.4	653
537	Doping by large-size-mismatched impurities: the microscopic origin of arsenic- or antimony-doped p-type zinc oxide. *Physical Review Letters*, **2004**, 92, 155504	7.4	549
536	Band Edge Electronic Structure of BiVO4: Elucidating the Role of the Bi s and V d Orbitals. *Chemistry of Materials*, **2009**, 21, 547-551	9.6	542
535	Intrinsic point defects and complexes in the quaternary kesterite semiconductor Cu2ZnSnS4. *Physical Review B*, **2010**, 81,	3.3	532
534	Crystal and electronic band structure of Cu2ZnSnX4 (X=S and Se) photovoltaic absorbers: First-principles insights. *Applied Physics Letters*, **2009**, 94, 041903	3.4	526
533	Role of metal d states in II-VI semiconductors. *Physical Review B*, **1988**, 37, 8958-8981	3.3	526
532	Nature of the band gap of In2O3 revealed by first-principles calculations and x-ray spectroscopy. *Physical Review Letters*, **2008**, 100, 167402	7.4	498
531	Design of Lead-Free Inorganic Halide Perovskites for Solar Cells via Cation-Transmutation. *Journal of the American Chemical Society*, **2017**, 139, 2630-2638	16.4	490
530	Kesterite Thin-Film Solar Cells: Advances in Materials Modelling of Cu2ZnSnS4. *Advanced Energy Materials*, **2012**, 2, 400-409	21.8	488

529	Predicted band-gap pressure coefficients of all diamond and zinc-blende semiconductors: Chemical trends. *Physical Review B*, **1999**, 60, 5404-5411	3.3	480
528	Giant and composition-dependent optical bowing coefficient in GaAsN alloys. *Physical Review Letters*, **1996**, 76, 664-667	7.4	478
527	Local-density-functional calculation of the pressure-induced metallization of BaSe and BaTe. *Physical Review Letters*, **1985**, 55, 1200-1203	7.4	476
526	Chemical trends of defect formation and doping limit in II-VI semiconductors: The case of CdTe. *Physical Review B*, **2002**, 66,	3.3	463
525	Effects of Ga addition to CuInSe2 on its electronic, structural, and defect properties. *Applied Physics Letters*, **1998**, 72, 3199-3201	3.4	420
524	Defect physics of the kesterite thin-film solar cell absorber Cu2ZnSnS4. *Applied Physics Letters*, **2010**, 96, 021902	3.4	405
523	Band offsets and optical bowings of chalcopyrites and Zn-based II-VI alloys. *Journal of Applied Physics*, **1995**, 78, 3846-3856	2.5	398
522	Self-regulation mechanism for charged point defects in hybrid halide perovskites. *Angewandte Chemie - International Edition*, **2015**, 54, 1791-4	16.4	394
521	Gas sensing in 2D materials. *Applied Physics Reviews*, **2017**, 4, 021304	17.3	381
520	Overcoming the doping bottleneck in semiconductors. *Computational Materials Science*, **2004**, 30, 337-348	3.2	377
519	A phenomenological model for systematization and prediction of doping limits in II-VI and I-III-VI2 compounds. *Journal of Applied Physics*, **1998**, 83, 3192-3196	2.5	372
518	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	2.5	360
517	Electronic structure and stability of quaternary chalcogenide semiconductors derived from cation cross-substitution of II-VI and I-III-VI2 compounds. *Physical Review B*, **2009**, 79,	3.3	359
516	Origin and enhancement of hole-induced ferromagnetism in first-row d0 semiconductors. *Physical Review Letters*, **2009**, 102, 017201	7.4	355
515	Compositional dependence of structural and electronic properties of Cu2ZnSn(S,Se)4 alloys for thin film solar cells. *Physical Review B*, **2011**, 83,	3.3	350
514	Van der Waals metal-semiconductor junction: Weak Fermi level pinning enables effective tuning of Schottky barrier. *Science Advances*, **2016**, 2, e1600069	14.3	338
513	Novel and Enhanced Optoelectronic Performances of Multilayer MoS2–WS2 Heterostructure Transistors. *Advanced Functional Materials*, **2014**, 24, 7025-7031	15.6	320
512	First-principles study of native defects in anatase TiO2. *Physical Review B*, **2006**, 73,	3.3	307

511	Valence band splittings and band offsets of AlN, GaN, and InN. *Applied Physics Letters*, **1996**, 69, 2719-2721	3.4	303
510	Effects of Na on the electrical and structural properties of CuInSe2. *Journal of Applied Physics*, **1999**, 85, 7214-7218	2.5	283
509	Band structure and fundamental optical transitions in wurtzite AlN. *Applied Physics Letters*, **2003**, 83, 5163-5165	3.4	282
508	Bipolar doping and band-gap anomalies in delafossite transparent conductive oxides. *Physical Review Letters*, **2002**, 88, 066405	7.4	280
507	First-principles statistical mechanics of structural stability of intermetallic compounds. *Physical Review B*, **1991**, 44, 512-544	3.3	274
506	Band structure engineering of semiconductors for enhanced photoelectrochemical water splitting: The case of TiO2. *Physical Review B*, **2010**, 82,	3.3	272
505	Stabilization of Ternary Compounds via Ordered Arrays of Defect Pairs. *Physical Review Letters*, **1997**, 78, 4059-4062	7.4	264
504	High-Performance Hydrogen Evolution from MoS2(1-x) P(x) Solid Solution. *Advanced Materials*, **2016**, 28, 1427-32	24	260
503	Electronic and structural anomalies in lead chalcogenides. *Physical Review B*, **1997**, 55, 13605-13610	3.3	259
502	The state and future prospects of kesterite photovoltaics. *Energy and Environmental Science*, **2013**, 6, 3171	35.4	256
501	Doping of ZnO by group-IB elements. *Applied Physics Letters*, **2006**, 89, 181912	3.4	251
500	Localization and percolation in semiconductor alloys: GaAsN vs GaAsP. *Physical Review B*, **1996**, 54, 17568-17576	3.3	249
499	First-principles calculation of alloy phase diagrams: The renormalized-interaction approach. *Physical Review B*, **1989**, 40, 3197-3231	3.3	244
498	Theoretical description of carrier mediated magnetism in cobalt doped ZnO. *Physical Review Letters*, **2008**, 100, 256401	7.4	240
497	Origins of band-gap renormalization in degenerately doped semiconductors. *Physical Review B*, **2008**, 78,	3.3	235
496	First-principles calculation of temperature-composition phase diagrams of semiconductor alloys. *Physical Review B*, **1990**, 41, 8240-8269	3.3	232
495	Total-energy and band-structure calculations for the semimagnetic Cd1-xMnxTe semiconductor alloy and its binary constituents. *Physical Review B*, **1987**, 35, 2340-2365	3.3	229
494	Wurtzite-derived polytypes of kesterite and stannite quaternary chalcogenide semiconductors. *Physical Review B*, **2010**, 82,	3.3	220

493	Theoretical study of the effects of isovalent coalloying of Bi and N in GaAs. *Physical Review B*, **2002**, 65,	3.3	219
492	Engineering Solar Cell Absorbers by Exploring the Band Alignment and Defect Disparity: The Case of Cu- and Ag-Based Kesterite Compounds. *Advanced Functional Materials*, **2015**, 25, 6733-6743	15.6	218
491	Band gaps and spin-orbit splitting of ordered and disordered AlxGa1-xAs and GaAsxSb1-x alloys. *Physical Review B*, **1989**, 39, 3279-3304	3.3	217
490	Band-gap narrowing in ordered and disordered semiconductor alloys. *Applied Physics Letters*, **1990**, 56, 662-664	3.4	216
489	Predicting two-dimensional boron-carbon compounds by the global optimization method. *Journal of the American Chemical Society*, **2011**, 133, 16285-90	16.4	209
488	Nitrogen solubility and induced defect complexes in epitaxial GaAs:N. *Physical Review Letters*, **2001**, 86, 1789-92	7.4	208
487	Simultaneous band-gap narrowing and carrier-lifetime prolongation of organic-inorganic trihalide perovskites. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 8910-5	11.5	199
486	Localization and anticrossing of electron levels in GaAs1□Nx alloys. *Physical Review B*, **1999**, 60, R11245-R11248	3.3	197
485	Influence of Defects and Synthesis Conditions on the Photovoltaic Performance of Perovskite Semiconductor CsSnI3. *Chemistry of Materials*, **2014**, 26, 6068-6072	9.6	194
484	Structure stability and carrier localization in CdX(X=S,Se,Te) semiconductors. *Physical Review B*, **2000**, 62, 6944-6947	3.3	192
483	Design of shallow acceptors in ZnO: First-principles band-structure calculations. *Physical Review B*, **2006**, 74,	3.3	190
482	Anomalous Alloy Properties in Mixed Halide Perovskites. *Journal of Physical Chemistry Letters*, **2014** , 5, 3625-31	6.4	188
481	Possible approach to overcome the doping asymmetry in wideband gap semiconductors. *Physical Review Letters*, **2007**, 98, 135506	7.4	184
480	Role of d orbitals in valence-band offsets of common-anion semiconductors. *Physical Review Letters* , **1987**, 59, 144-147	7.4	184
479	Microscopic origin of the phenomenological equilibrium "Doping limit Rule" in n-type III-V semiconductors. *Physical Review Letters*, **2000**, 84, 1232-5	7.4	180
478	Electrically benign behavior of grain boundaries in polycrystalline CuInSe2 films. *Physical Review Letters*, **2007**, 99, 235504	7.4	176
477	Layer-dependent electrical and optoelectronic responses of ReSe2 nanosheet transistors. *Nanoscale*, **2014**, 6, 7226-31	7.7	170
476	Electronic structure and phase stability of MgO, ZnO, CdO, and related ternary alloys. *Physical Review B*, **2008**, 77,	3.3	167

475	Relationships between the band gaps of the zinc-blende and wurtzite modifications of semiconductors. *Physical Review B*, **1994**, 50, 2715-2718	3.3	167
474	Predicting the spin-lattice order of frustrated systems from first principles. *Physical Review B*, **2011**, 84,	3.3	166
473	Fundamental optical transitions in GaN. *Applied Physics Letters*, **1996**, 68, 2784-2786	3.4	165
472	Revised ab initio natural band offsets of all group IV, II-VI, and III-V semiconductors. *Applied Physics Letters*, **2009**, 94, 212109	3.4	162
471	Predicting synthesizability. *Journal Physics D: Applied Physics*, **2019**, 52,	3	161
470	Doping properties of monoclinic BiVO4 studied by first-principles density-functional theory. *Physical Review B*, **2011**, 83,	3.3	161
469	Resonant hole localization and anomalous optical bowing in InGaN alloys. *Applied Physics Letters*, **1999**, 74, 1842-1844	3.4	159
468	Spin-orbit coupling and ion displacements in multiferroic TbMnO3. *Physical Review Letters*, **2008**, 101, 037209	7.4	158
467	Effective band gap narrowing of anatase TiO2 by strain along a soft crystal direction. *Applied Physics Letters*, **2010**, 96, 221901	3.4	154
466	Doping asymmetry in wide-bandgap semiconductors: Origins and solutions. *Physica Status Solidi (B): Basic Research*, **2008**, 245, 641-652	1.3	153
465	Structural diversity and electronic properties of Cu2SnX3 (X=S, Se): A first-principles investigation. *Physical Review B*, **2011**, 84,	3.3	152
464	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	6.4	150
463	Piezophototronic Effect in Single-Atomic-Layer MoS for Strain-Gated Flexible Optoelectronics. *Advanced Materials*, **2016**, 28, 8463-8468	24	149
462	First-principles study of cation distribution in eighteen closed-shell AIIB2IIIO4 and AIVB2IIO4 spinel oxides. *Physical Review B*, **2001**, 63,	3.3	148
461	Band gaps of GaPN and GaAsN alloys. *Applied Physics Letters*, **1997**, 70, 3558-3560	3.4	145
460	Ground-state structures and the random-state energy of the Madelung lattice. *Physical Review B*, **1990**, 42, 11388-11391	3.3	145
459	Calculated spin-orbit splitting of all diamondlike and zinc-blende semiconductors: Effects of p1⁄2 local orbitals and chemical trends. *Physical Review B*, **2004**, 70,	3.3	142
458	Abundance of CuZn + SnZn and 2CuZn + SnZn defect clusters in kesterite solar cells. *Applied Physics Letters*, **2012**, 101, 223901	3.4	140

457	First-principles calculations of the phase diagrams of noble metals: Cu-Au, Cu-Ag, and Ag-Au. *Physical Review B*, **1987**, 36, 4163-4185	3.3	138
456	Origin of the unusually large band-gap bowing and the breakdown of the band-edge distribution rule in the SnxGe1 alloys. *Physical Review B*, **2008**, 78,	3.3	136
455	Structural, magnetic, and electronic properties of the Co-Fe-Al oxide spinel system: Density-functional theory calculations. *Physical Review B*, **2007**, 76,	3.3	134
454	Hydrogen passivation effect in nitrogen-doped ZnO thin films. *Applied Physics Letters*, **2005**, 86, 122107	3.4	134
453	Pseudopotential plane-wave calculations for ZnS. *Physical Review B*, **1991**, 43, 2213-2217	3.3	134
452	Optical properties of zinc-blende semiconductor alloys: Effects of epitaxial strain and atomic ordering. *Physical Review B*, **1994**, 49, 14337-14351	3.3	132
451	Linearized augmented-plane-wave calculation of the electronic structure and total energy of tungsten. *Physical Review B*, **1985**, 32, 7792-7797	3.3	132
450	High thermoelectric performance in copper telluride. *NPG Asia Materials*, **2015**, 7, e210-e210	10.3	131
449	Composition dependence of interband transition intensities in GaPN, GaAsN, and GaPAs alloys. *Physical Review B*, **1997**, 56, 10233-10240	3.3	130
448	Double-hole-mediated coupling of dopants and its impact on band gap engineering in TiO2. *Physical Review Letters*, **2011**, 106, 066801	7.4	126
447	Origin of the structural and magnetic anomalies of the layered compound SrFeO2: a density functional investigation. *Physical Review Letters*, **2008**, 100, 167207	7.4	126
446	Dependence of the optical properties of semiconductor alloys on the degree of long-range order. *Applied Physics Letters*, **1993**, 62, 1937-1939	3.4	125
445	Phase control of CuxTe film and its effects on CdS/CdTe solar cell. *Thin Solid Films*, **2007**, 515, 5798-5803	2.2	123
444	Ab initio all-electron calculation of absolute volume deformation potentials of IV-IV, III-V, and II-VI semiconductors: The chemical trends. *Physical Review B*, **2006**, 73,	3.3	123
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442	Realizing a SnO2-based ultraviolet light-emitting diode via breaking the dipole-forbidden rule. *NPG Asia Materials*, **2012**, 4, e30-e30	10.3	119
441	Engineering Grain Boundaries in Cu2ZnSnSe4 for Better Cell Performance: A First-Principle Study. *Advanced Energy Materials*, **2014**, 4, 1300712	21.8	118
440	Phenomenological band structure model of magnetic coupling in semiconductors. *Solid State Communications*, **2006**, 138, 353-358	1.6	117

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435	Electronic Structure and Optical Properties of □CH3NH3PbBr3 Perovskite Single Crystal. *Journal of Physical Chemistry Letters*, **2015**, 6, 4304-8	6.4	113
434	Structure-derived electronic and optical properties of transparent conducting oxides. *Physical Review B*, **2005**, 71,	3.3	113
433	Electron-induced stabilization of ferromagnetism in Ga1□GdxN. *Physical Review B*, **2005**, 72,	3.3	113
432	Towards direct-gap silicon phases by the inverse band structure design approach. *Physical Review Letters*, **2013**, 110, 118702	7.4	112
431	Electronic, structural, and magnetic effects of 3d transition metals in hematite. *Journal of Applied Physics*, **2010**, 107, 123712	2.5	111
430	Band-structure anomalies of the chalcopyrite semiconductors CuGaX2 versus AgGaX2 (X=S and Se) and their alloys. *Physical Review B*, **2007**, 75,	3.3	111
429	Two-Dimensional SiS Layers with Promising Electronic and Optoelectronic Properties: Theoretical Prediction. *Nano Letters*, **2016**, 16, 1110-7	11.5	110
428	Design of I2□IV□VI4 Semiconductors through Element Substitution: The Thermodynamic Stability Limit and Chemical Trend. *Chemistry of Materials*, **2014**, 26, 3411-3417	9.6	109
427	Intrinsic Instability of the Hybrid Halide Perovskite Semiconductor CH 3 NH 3 PbI 3 *. *Chinese Physics Letters*, **2018**, 35, 036104	1.8	107
426	Origin of the variation of exciton binding energy in semiconductors. *Physical Review Letters*, **2013**, 110, 016402	7.4	107
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421	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	7.4	96
420	Native defect-induced multifarious magnetism in nonstoichiometric cuprous oxide: First-principles study of bulk and surface properties of Cu2O. *Physical Review B*, **2009**, 79,	3.3	96
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418	Effect of copassivation of Cl and Cu on CdTe grain boundaries. *Physical Review Letters*, **2008**, 101, 155501	7.4	95
417	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	3.3	93
416	Breakdown of the band-gap-common-cation rule: The origin of the small band gap of InN. *Physical Review B*, **2003**, 67,	3.3	93
415	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,	3.3	92
414	Crystal and electronic structures of CuxS solar cell absorbers. *Applied Physics Letters*, **2012**, 100, 061906	3.4	91
413	Self-Regulation Mechanism for Charged Point Defects in Hybrid Halide Perovskites. *Angewandte Chemie*, **2015**, 127, 1811-1814	3.6	87
412	Effects of hydrogen on the electronic properties of dilute GaAsN alloys. *Physical Review Letters*, **2002**, 89, 086403	7.4	87
411	Majority Representation of Alloy Electronic States. *Physical Review Letters*, **1998**, 80, 4725-4728	7.4	87
410	Evolution of alloy properties with long-range order. *Physical Review Letters*, **1992**, 69, 3766-3769	7.4	87
409	Na-Diffusion Enhanced p-type Conductivity in Cu(In,Ga)Se2: A New Mechanism for Efficient Doping in Semiconductors. *Advanced Energy Materials*, **2016**, 6, 1601191	21.8	86
408	Electronic structure of ZnO:GaN compounds: Asymmetric bandgap engineering. *Physical Review B*, **2008**, 78,	3.3	85
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406	Disorder effects on the density of states of the II-VI semiconductor alloys Hg0.5Cd0.5Te, Cd0.5Zn0.5Te, and Hg0.5Zn0.5Te. *Physical Review B*, **1991**, 43, 1662-1677	3.3	85
405	High Performance Electrocatalytic Reaction of Hydrogen and Oxygen on Ruthenium Nanoclusters. *ACS Applied Materials & Interfaces*, **2017**, 9, 3785-3791	9.5	84
404	Tunable Polarity Behavior and Self-Driven Photoswitching in p-WSe2/n-WS2 Heterojunctions. *Small*, **2015**, 11, 5430-8	11	84

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400	Electronic structure of ordered and disordered Cu3Au and Cu3Pd. *Physical Review B*, **1992**, 45, 10314-10330	3.3	83
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398	Band Structure Engineering of CsAgBiBr Perovskite through Order-Disordered Transition: A First-Principle Study. *Journal of Physical Chemistry Letters*, **2018**, 9, 31-35	6.4	82
397	Interplay between Order and Disorder in the High Performance of Amorphous Transparent Conducting Oxides. *Chemistry of Materials*, **2009**, 21, 5119-5124	9.6	80
396	Density-functional theory study of the effects of atomic impurity on the band edges of monoclinic WO3. *Physical Review B*, **2008**, 77,	3.3	80
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392	Band structure and stability of zinc-blende-based semiconductor polytypes. *Physical Review B*, **1999**, 59, R2478-R2481	3.3	75
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388	Review on first-principles study of defect properties of CdTe as a solar cell absorber. *Semiconductor Science and Technology*, **2016**, 31, 083002	1.8	73
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386	Defect properties of CuInSe2 and CuGaSe2. *Journal of Physics and Chemistry of Solids*, **2005**, 66, 1994-1999	3.9	73

385	A Unified Understanding of the Thickness-Dependent Bandgap Transition in Hexagonal Two-Dimensional Semiconductors. *Journal of Physical Chemistry Letters*, **2016**, 7, 597-602	6.4	72
384	Origin of long-range ferromagnetic ordering in metal-organic frameworks with antiferromagnetic dimeric-Cu(II) building units. *Journal of the American Chemical Society*, **2012**, 134, 17286-90	16.4	72
383	Strain control of magnetism in graphene decorated by transition-metal atoms. *Physical Review B*, **2011**, 84,	3.3	72
382	Kesterite Successes, Ongoing Work, and Challenges: A Perspective From Vacuum Deposition. *IEEE Journal of Photovoltaics*, **2013**, 3, 439-445	3.7	71
381	Oxygen-vacancy mediated adsorption and reactions of molecular oxygen on the ZnO(101□0) surface. *Physical Review B*, **2005**, 72,	3.3	71
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377	Structural motifs in oxidized graphene: A genetic algorithm study based on density functional theory. *Physical Review B*, **2010**, 82,	3.3	70
376	Design of shallow donor levels in diamond by isovalent-donor coupling. *Physical Review Letters*, **2003**, 91, 126406	7.4	70
375	Band-gap bowing coefficients in large size-mismatched II-VI alloys: first-principles calculations. *Physical Review B*, **2006**, 74,	3.3	69
374	Electronic origins of the magnetic phase transitions in zinc-blende Mn chalcogenides. *Physical Review B*, **1993**, 48, 6111-6115	3.3	69
373	First-principles study on the effective masses of zinc-blend-derived Cu2ZnⅣⅥ4 (IV = Sn, Ge, Si and VI = S, Se). *Journal of Applied Physics*, **2012**, 112, 093717	2.5	68
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