

Su-Huai Wei

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Energetic Cocrystallization as the Most Significant Crystal Engineering Way to Create New Energetic Materials. <i>Crystal Growth and Design</i> , 2022 , 22, 954-970	3.5	2
545	Clarification of the relative magnitude of exciton binding energies in ZnO and SnO ₂ . <i>Applied Physics Letters</i> , 2022 , 120, 042105	3.4	3
544	General Model for Defect Dynamics in Ionizing-Irradiated SiO ₂ -Si Structures.. <i>Small</i> , 2022 , e2107516	11	2
543	Band gap anomaly in cuprous halides. <i>Computational Materials Science</i> , 2022 , 203, 111157	3.2	1
542	Origin of Efficiency Enhancement by Lattice Expansion in Hybrid-Perovskite Solar Cells.. <i>Physical Review Letters</i> , 2022 , 128, 136401	7.4	5
541	Universal Theory and Basic Rules of Strain-Dependent Doping Behaviors in Semiconductors. <i>Chinese Physics Letters</i> , 2021 , 38, 087103	1.8	0
540	Approach to achieving a p-type transparent conducting oxide: Doping of bismuth-alloyed Ga ₂ O ₃ with a strongly correlated band edge state. <i>Physical Review B</i> , 2021 , 103,	3.3	7
539	Interface Engineering of Cu(In,Ga)Se Solar Cells by Optimizing Cd- and Zn-Chalcogenide Alloys as the Buffer Layer. <i>ACS Applied Materials & Interfaces</i> , 2021 , 13, 15237-15245	9.5	3
538	Polymorph-Dependent Initial Thermal Decay Mechanism of Energetic Materials: A Case of 1,3,5,7-Tetranitro-1,3,5,7-Tetrazocane. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 10057-10067	3.8	4
537	Electron donation of non-oxide supports boosts O activation on nano-platinum catalysts. <i>Nature Communications</i> , 2021 , 12, 2741	17.4	19
536	Optimization of Doping CdTe with Group-V Elements: A First-Principles Study. <i>Physical Review Applied</i> , 2021 , 15,	4.3	2
535	Enhancing magnetic dipole emission in Eu-doped SrMO ₃ (M=Ti,Zr,Hf): First-principles calculations. <i>Physical Review B</i> , 2021 , 103,	3.3	1
534	Strong Coupled Magnetic and Electric Ordering in Monolayer of Metal Thio(seleno)phosphates. <i>Chinese Physics Letters</i> , 2021 , 38, 077501	1.8	7
533	First-principles study of defect control in thin-film solar cell materials. <i>Science China: Physics, Mechanics and Astronomy</i> , 2021 , 64, 1	3.6	7
532	Enhanced performance of Se-alloyed CdTe solar cells: The role of Se-segregation on the grain boundaries. <i>Journal of Applied Physics</i> , 2021 , 129, 024501	2.5	4
531	More Se Vacancies in Sb Se under Se-Rich Conditions: An Abnormal Behavior Induced by Defect-Correlation in Compensated Compound Semiconductors. <i>Small</i> , 2021 , 17, e2102429	11	7
530	Origin of anomalous band-gap bowing in two-dimensional tin-lead mixed perovskite alloys. <i>Physical Review B</i> , 2021 , 104,	3.3	2

529	Perspective on the band structure engineering and doping control of transparent conducting materials. <i>Applied Physics Letters</i> , 2021 , 119, 070502	3.4	1
528	Group velocity matters for accurate prediction of phonon-limited carrier mobility*. <i>Chinese Physics B</i> , 2021 , 30, 087201	1.2	
527	Decoupling of the Electrical and Thermal Transports in Strongly Coupled Interlayer Materials. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 7832-7839	6.4	1
526	Atomic-scale understanding on the physics and control of intrinsic point defects in lead halide perovskites. <i>Applied Physics Reviews</i> , 2021 , 8, 031302	17.3	15
525	Flat bands in twisted bilayers of polar two-dimensional semiconductors. <i>Physical Review Materials</i> , 2021 , 5,	3.2	3
524	Design of Multifunctional Quaternary Metal-Halide Perovskite Compounds Based on Cation/Anion Co-Ordering. <i>Chemistry of Materials</i> , 2020 , 32, 5949-5957	9.6	3
523	Defect Dynamic Model of the Synergistic Effect in Neutron- and β -Ray-Irradiated Silicon NPN Transistors. <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 29993-29998	9.5	3
522	Unconventional deformation potential and half-metallicity in zigzag nanoribbons of 2D-Xenes. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 7294-7299	3.6	2
521	Band-Structure Engineering of $\text{ZnxCd}_{1-x}\text{SySe}_{1-y}$ Quaternary Alloys as the Window Layer for CdTe Solar Cells. <i>Physical Review Applied</i> , 2020 , 13,	4.3	1
520	Formation of Bloch Flat Bands in Polar Twisted Bilayers without Magic Angles. <i>Physical Review Letters</i> , 2020 , 124, 086401	7.4	29
519	First-principles study of electronic and diffusion properties of intrinsic defects in 4H-SiC. <i>Journal of Applied Physics</i> , 2020 , 127, 085702	2.5	17
518	Strain induced spin-splitting and half-metallicity in antiferromagnetic bilayer silicene under bending. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 11567-11571	3.6	6
517	Chemical trend of a Cu impurity in Zn chalcogenides. <i>Physical Review B</i> , 2020 , 101,	3.3	2
516	Accurate and effective computation of the multi-phonon nonradiative transition. <i>Science China: Physics, Mechanics and Astronomy</i> , 2020 , 63, 1	3.6	
515	Functionalizing Two-Dimensional Materials for Energy Applications 2020 , 567-603		1
514	ToF-SIMS Investigation of the Initial Stages of $\text{MeCpPt}(\text{CH}_3)_3$ Adsorption and Decomposition on Nickel Oxide Surfaces: Exploring the Role and Location of the Ligands. <i>Organometallics</i> , 2020 , 39, 1024-1034	3.8	4
513	Theoretical investigation of halide perovskites for solar cell and optoelectronic applications. <i>Chinese Physics B</i> , 2020 , 29, 108401	1.2	7
512	Origin of the Stability and Transition from Anionic to Cationic Surface Ligand Passivation of All-Inorganic Cesium Lead Halide Perovskite Nanocrystals. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 652-658	6.4	21

511	Designing Dirac semimetals with a honeycomb Na ₃ Bi-lattice via isovalent cation substitution. <i>Journal of Materials Chemistry C</i> , 2020 , 8, 1257-1264	7.1	2
510	Gamma-ray irradiation-induced oxidation and disproportionation at the amorphous SiO ₂ /Si interfaces. <i>Journal of Materials Chemistry C</i> , 2020 , 8, 17065-17073	7.1	1
509	Origin of Irradiation Synergistic Effects in Silicon Bipolar Transistors. <i>ACS Applied Electronic Materials</i> , 2020 , 2, 3783-3793	4	4
508	Self-Catalyzed Sensitization of CuO Nanowires via a Solvent-free Click Reaction. <i>Langmuir</i> , 2020 , 36, 14539-14545	7.1	1
507	Searching for stable perovskite solar cell materials using materials genome techniques and high-throughput calculations. <i>Journal of Materials Chemistry C</i> , 2020 , 8, 12012-12035	7.1	11
506	Review of the Intermolecular Interactions in Energetic Molecular Cocrystals. <i>Crystal Growth and Design</i> , 2020 , 20, 7065-7079	3.5	22
505	Realistic dimension-independent approach for charged-defect calculations in semiconductors. <i>Physical Review B</i> , 2020 , 101,	3.3	14
504	Achieving High Volumetric Lithium Storage Capacity in Compact Carbon Materials with Controllable Nitrogen Doping. <i>Advanced Functional Materials</i> , 2019 , 29, 1807441	15.6	24
503	Origin of High-TC Ferromagnetism in Isovalent-Doped III-V Semiconductors. <i>Physical Review Applied</i> , 2019 , 11,	4.3	8
502	UV-ozone induced surface passivation to enhance the performance of Cu ₂ ZnSnS ₄ solar cells. <i>Solar Energy Materials and Solar Cells</i> , 2019 , 200, 109892	6.4	9
501	Alloy-induced phase transition and enhanced photovoltaic performance: the case of Cs ₃ Bi ₂ I ₉ Br _x perovskite solar cells. <i>Journal of Materials Chemistry A</i> , 2019 , 7, 8818-8825	13	45
500	Mechanism of Synergistic Effects of Neutron- and Gamma-Ray-Radiated PNP Bipolar Transistors. <i>ACS Applied Electronic Materials</i> , 2019 , 1, 538-547	4	10
499	Origin of Deep Be Acceptor Levels in Nitride Semiconductors: The Roles of Chemical and Strain Effects. <i>Physical Review Applied</i> , 2019 , 11,	4.3	8
498	Formation of DY center as n-type limiting defects in octahedral semiconductors: the case of Bi-doped hybrid halide perovskites. <i>Journal of Materials Chemistry C</i> , 2019 , 7, 4230-4234	7.1	33
497	Materials Design of Solar Cell Absorbers Beyond Perovskites and Conventional Semiconductors via Combining Tetrahedral and Octahedral Coordination. <i>Advanced Materials</i> , 2019 , 31, e1806593	24	29
496	Origin of the anomalous trends in band alignment of GaX/ZnGeX ₂ (X = N, P, As, Sb) heterojunctions. <i>Journal of Semiconductors</i> , 2019 , 40, 042102	2.3	4
495	Predicting synthesizability. <i>Journal Physics D: Applied Physics</i> , 2019 , 52,	3	161
494	Transition from Positive to Negative Photoconductance in Doped Hybrid Perovskite Semiconductors. <i>Advanced Optical Materials</i> , 2019 , 7, 1900865	8.1	27

493	First-principles study of the band gap tuning and doping control in CdSe x Te _{1-x} alloy for high efficiency solar cell. <i>Chinese Physics B</i> , 2019 , 28, 086106	1.2	25
492	Revisit of the band gaps of rutile SnO ₂ and TiO ₂ : a first-principles study. <i>Journal of Semiconductors</i> , 2019 , 40, 092101	2.3	8
491	Nanowire Quantum Dot Surface Engineering for High Temperature Single Photon Emission. <i>ACS Nano</i> , 2019 , 13, 13492-13500	16.7	13
490	Enabling visible-light absorption and p-type doping in In ₂ O ₃ by adding Bi. <i>Physical Review Materials</i> , 2019 , 3,	3.2	2
489	Design of p-type transparent conductors from inverted band structure: The case of inorganic metal halide perovskites. <i>Physical Review Materials</i> , 2019 , 3,	3.2	16
488	Hole-Induced Spontaneous Mutual Annihilation of Dislocation Pairs. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 7421-7425	6.4	
487	A systematic study of the negative thermal expansion in zinc-blende and diamond-like semiconductors. <i>New Journal of Physics</i> , 2019 , 21, 123015	2.9	3
486	Stable Bandgap-Tunable Hybrid Perovskites with Alloyed Pb-Ba Cations for High-Performance Photovoltaic Applications. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 59-66	6.4	33
485	The Coulomb interaction in van der Waals heterostructures. <i>Science China: Physics, Mechanics and Astronomy</i> , 2019 , 62, 1	3.6	19
484	Effective and Noneffective Recombination Center Defects in Cu ₂ ZnSnS ₄ : Significant Difference in Carrier Capture Cross Sections. <i>Chemistry of Materials</i> , 2019 , 31, 826-833	9.6	44
483	Intrinsic Instability of the Hybrid Halide Perovskite Semiconductor CH ₃ NH ₃ PbI ₃ *. <i>Chinese Physics Letters</i> , 2018 , 35, 036104	1.8	107
482	Modulation of electronic and magnetic properties of edge hydrogenated armchair phosphorene nanoribbons by transition metal adsorption. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 12916-12922	3.6	9
481	Tuning the optical bandgap in multi-cation compound transparent conducting-oxides: The examples of In ₂ ZnO ₄ and In ₄ Sn ₃ O ₁₂ . <i>Journal of Applied Physics</i> , 2018 , 123, 055704	2.5	1
480	Design of n-Type Transparent Conducting Oxides: The Case of Transition Metal Doping in In ₂ O ₃ . <i>Advanced Electronic Materials</i> , 2018 , 4, 1700553	6.4	32
479	Comment on "Fundamental Resolution of Difficulties in the Theory of Charged Point Defects in Semiconductors". <i>Physical Review Letters</i> , 2018 , 120, 039601	7.4	5
478	Manipulation of cation combinations and configurations of halide double perovskites for solar cell absorbers. <i>Journal of Materials Chemistry A</i> , 2018 , 6, 1809-1815	13	50
477	CsCu ₅ Se ₃ : A Copper-Rich Ternary Chalcogenide Semiconductor with Nearly Direct Band Gap for Photovoltaic Application. <i>Chemistry of Materials</i> , 2018 , 30, 1121-1126	9.6	23
476	First-principles study of alloying effects on fluorine incorporation in Al _x Ga _{1-x} N alloys. <i>Journal Physics D: Applied Physics</i> , 2018 , 51, 065108	3	7

475	Origin of charge compensation and its effect on the stability of oxide cathodes for Li-ion batteries: The case of orthosilicates. <i>Electrochimica Acta</i> , 2018 , 270, 409-416	6.7	9
474	Interface Engineering of Graphene/CH ₃ NH ₃ PbI ₃ Heterostructure for Novel p-n Structural Perovskites Solar Cells. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 17228-17237	3.8	15
473	Influence of defects on the thermoelectricity in SnSe: A comprehensive theoretical study. <i>Physical Review B</i> , 2018 , 97,	3.3	33
472	The stabilization mechanism and size effect of nonpolar-to-polar crystallography facet tailored ZnO nano/micro rods via a top-down strategy. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 18455-18462	3.6	3
471	Band Structure Engineering of CsAgBiBr Perovskite through Order-Disordered Transition: A First-Principle Study. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 31-35	6.4	82
470	Highly-anisotropic optical and electrical properties in layered SnSe. <i>Nano Research</i> , 2018 , 11, 554-564	10	77
469	Magnetic origin of phase stability in cubic ϵ -MoN. <i>Applied Physics Letters</i> , 2018 , 113, 221901	3.4	6
468	Band structure engineering and defect control of oxides for energy applications. <i>Chinese Physics B</i> , 2018 , 27, 117104	1.2	13
467	Unified theory of direct or indirect band-gap nature of conventional semiconductors. <i>Physical Review B</i> , 2018 , 98,	3.3	26
466	Photocorrosion-Limited Maximum Efficiency of Solar Photoelectrochemical Water Splitting. <i>Physical Review Applied</i> , 2018 , 10,	4.3	28
465	Functionalizing Two-Dimensional Materials for Energy Applications 2018 , 1-37		
464	Distinct Excitonic Circular Dichroism between Wurtzite and Zincblende CdSe Nanoplatelets. <i>Nano Letters</i> , 2018 , 18, 6665-6671	11.5	45
463	Atomic-Ordering-Induced Quantum Phase Transition between Topological Crystalline Insulator and Z ₂ Topological Insulator. <i>Chinese Physics Letters</i> , 2018 , 35, 057301	1.8	4
462	High-throughput screening of chalcogenide single perovskites by first-principles calculations for photovoltaics. <i>Journal Physics D: Applied Physics</i> , 2018 , 51, 474003	3	25
461	Preface for Special Topic: Earth abundant materials in solar cells. <i>APL Materials</i> , 2018 , 6, 084401	5.7	2
460	Origin of the stability of two-dimensional perovskites: a first-principles study. <i>Journal of Materials Chemistry A</i> , 2018 , 6, 14949-14955	13	54
459	Design of Lead-Free Inorganic Halide Perovskites for Solar Cells via Cation-Transmutation. <i>Journal of the American Chemical Society</i> , 2017 , 139, 2630-2638	16.4	490
458	High Performance Electrocatalytic Reaction of Hydrogen and Oxygen on Ruthenium Nanoclusters. <i>ACS Applied Materials & Interfaces</i> , 2017 , 9, 3785-3791	9.5	84

457	Optical and fundamental band gaps disparity in transparent conducting oxides: new findings for the [Formula: see text] and [Formula: see text] systems. <i>Journal of Physics Condensed Matter</i> , 2017 , 29, 085501	1.8	9
456	Antimony Diffusion in CdTe. <i>IEEE Journal of Photovoltaics</i> , 2017 , 7, 870-873	3.7	9
455	Gas sensing in 2D materials. <i>Applied Physics Reviews</i> , 2017 , 4, 021304	17.3	381
454	Earth-Abundant and Non-Toxic SiX (X = S, Se) Monolayers as Highly Efficient Thermoelectric Materials. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 123-128	3.8	28
453	Synthesis of Cs ₂ AgSbCl ₆ and improved optoelectronic properties of Cs ₂ AgSbCl ₆ /TiO ₂ heterostructure driven by the interface effect for lead-free double perovskites solar cells. <i>Applied Physics Letters</i> , 2017 , 111, 151602	3.4	41
452	Exploring Emerging Photovoltaic Materials Beyond Perovskite: The Case of Skutterudite. <i>Chemistry of Materials</i> , 2017 , 29, 9429-9435	9.6	13
451	Inhomogeneous strain-induced half-metallicity in bent zigzag graphene nanoribbons. <i>Npj Computational Materials</i> , 2017 , 3,	10.9	24
450	Microscopic mechanism of the tunable band gap in potassium-doped few-layer black phosphorus. <i>Physical Review B</i> , 2017 , 96,	3.3	13
449	Self-compensation in arsenic doping of CdTe. <i>Scientific Reports</i> , 2017 , 7, 4563	4.9	37
448	Carrier providers or killers: The case of Cu defects in CdTe. <i>Applied Physics Letters</i> , 2017 , 111, 042106	3.4	17
447	Origin of polymorphism of the two-dimensional group-IV monochalcogenides. <i>Physical Review B</i> , 2017 , 96,	3.3	16
446	Enhanced Electrical and Optoelectronic Characteristics of Few-Layer Type-II SnSe/MoS van der Waals Heterojunctions. <i>ACS Applied Materials & Interfaces</i> , 2017 , 9, 42149-42155	9.5	40
445	Nonisovalent Si-III-V and Si-II-VI alloys: Covalent, ionic, and mixed phases. <i>Physical Review B</i> , 2017 , 96,	3.3	1
444	Prediction of Ideal Topological Semimetals with Triply Degenerate Points in the NaCu ₃ Te ₂ Family. <i>Physical Review Letters</i> , 2017 , 119, 256402	7.4	29
443	Na-Diffusion Enhanced p-type Conductivity in Cu(In,Ga)Se ₂ : A New Mechanism for Efficient Doping in Semiconductors. <i>Advanced Energy Materials</i> , 2016 , 6, 1601191	21.8	86
442	Phosphorus Diffusion Mechanisms and Deep Incorporation in Polycrystalline and Single-Crystalline CdTe. <i>Physical Review Applied</i> , 2016 , 5,	4.3	20
441	Review on first-principles study of defect properties of CdTe as a solar cell absorber. <i>Semiconductor Science and Technology</i> , 2016 , 31, 083002	1.8	73
440	Simultaneous band-gap narrowing and carrier-lifetime prolongation of organic-inorganic trihalide perovskites. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016 , 113, 8910-5	11.5	199

439	Van der Waals metal-semiconductor junction: Weak Fermi level pinning enables effective tuning of Schottky barrier. <i>Science Advances</i> , 2016 , 2, e1600069	14.3	338
438	Non-Radiative Carrier Recombination Enhanced by Two-Level Process: A First-Principles Study. <i>Scientific Reports</i> , 2016 , 6, 21712	4.9	54
437	High-Performance Hydrogen Evolution from MoS ₂ (1-x)P(x) Solid Solution. <i>Advanced Materials</i> , 2016 , 28, 1427-32	24	260
436	A Unified Understanding of the Thickness-Dependent Bandgap Transition in Hexagonal Two-Dimensional Semiconductors. <i>Journal of Physical Chemistry Letters</i> , 2016 , 7, 597-602	6.4	72
435	Stabilizing Perovskite Structures by Tuning Tolerance Factor: Formation of Formamidinium and Cesium Lead Iodide Solid-State Alloys. <i>Chemistry of Materials</i> , 2016 , 28, 284-292	9.6	1186
434	Two-Dimensional SiS Layers with Promising Electronic and Optoelectronic Properties: Theoretical Prediction. <i>Nano Letters</i> , 2016 , 16, 1110-7	11.5	110
433	Air Passivation of Chalcogen Vacancies in Two-Dimensional Semiconductors. <i>Angewandte Chemie</i> , 2016 , 128, 977-980	3.6	10
432	Air Passivation of Chalcogen Vacancies in Two-Dimensional Semiconductors. <i>Angewandte Chemie - International Edition</i> , 2016 , 55, 965-8	16.4	67
431	Polymerization of defect states at dislocation cores in InAs. <i>Journal of Applied Physics</i> , 2016 , 119, 045706	2.5	5
430	Wild band edges: The role of bandgap grading and band-edge fluctuations in high-efficiency chalcogenide devices 2016 ,		10
429	Metal compound semiconductors functionalized by polymers and their photosensitive properties. <i>Applied Physics Reviews</i> , 2016 , 3, 041306	17.3	3
428	First-principles study of roles of Cu and Cl in polycrystalline CdTe. <i>Journal of Applied Physics</i> , 2016 , 119, 045104	2.5	31
427	Effect of intermixing at CdS/CdTe interface on defect properties. <i>Applied Physics Letters</i> , 2016 , 109, 042105	3.05	6
426	Suppress carrier recombination by introducing defects: The case of Si solar cell. <i>Applied Physics Letters</i> , 2016 , 108, 022101	3.4	18
425	Origin of the Distinct Diffusion Behaviors of Cu and Ag in Covalent and Ionic Semiconductors. <i>Physical Review Letters</i> , 2016 , 117, 165901	7.4	16
424	Piezophototronic Effect in Single-Atomic-Layer MoS for Strain-Gated Flexible Optoelectronics. <i>Advanced Materials</i> , 2016 , 28, 8463-8468	24	149
423	Fast self-diffusion of ions in CH ₃ NH ₃ PbI ₃ : the interstitially mechanism versus vacancy-assisted mechanism. <i>Journal of Materials Chemistry A</i> , 2016 , 4, 13105-13112	13	53
422	Ordering-induced direct-to-indirect band gap transition in multication semiconductor compounds. <i>Physical Review B</i> , 2015 , 91,	3.3	17

421	Effects of deposition termination on Cu ₂ ZnSnSe ₄ device characteristics. <i>Thin Solid Films</i> , 2015 , 582, 184-187	2.7	27
420	First-principles multiple-barrier diffusion theory: The case study of interstitial diffusion in CdTe. <i>Physical Review B</i> , 2015 , 91,	3.3	25
419	Stability and electronic structure of the low- κ grain boundaries in CdTe: a density functional study. <i>New Journal of Physics</i> , 2015 , 17, 013027	2.9	25
418	Device Performance of the Mott Insulator LaVO ₃ as a Photovoltaic Material. <i>Physical Review Applied</i> , 2015 , 3,	4.3	54
417	Interlayer coupling and optoelectronic properties of ultrathin two-dimensional heterostructures based on graphene, MoS ₂ and WS ₂ . <i>Journal of Materials Chemistry C</i> , 2015 , 3, 5467-5473	7.1	73
416	Origin of the structural diversity of M ₂ O ₃ (M = Al, Ga, In). <i>Computational Materials Science</i> , 2015 , 104, 35-39	3.2	1
415	Origin of High Electronic Quality in Structurally Disordered CH ₃ NH ₃ PbI ₃ and the Passivation Effect of Cl and O at Grain Boundaries. <i>Advanced Electronic Materials</i> , 2015 , 1, 1500044	6.4	150
414	Electronic Structure and Optical Properties of $\sqrt{2}\times\sqrt{2}$ CH ₃ NH ₃ PbBr ₃ Perovskite Single Crystal. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 4304-8	6.4	113
413	Enhanced p-type dopability of P and As in CdTe using non-equilibrium thermal processing. <i>Journal of Applied Physics</i> , 2015 , 118, 025102	2.5	42
412	Chemical trends of stability and band alignment of lattice-matched II-VI/III-V semiconductor interfaces. <i>Physical Review B</i> , 2015 , 91,	3.3	16
411	High thermoelectric performance in copper telluride. <i>NPG Asia Materials</i> , 2015 , 7, e210-e210	10.3	131
410	O-O bonding stabilized zinc vacancy as origin of p-type doping on $\sqrt{2}\times\sqrt{2}$ ZnO grain boundary. <i>Journal of Applied Physics</i> , 2015 , 118, 045708	2.5	6
409	Monitoring the stability of organometallic perovskite thin films. <i>Journal of Materials Chemistry A</i> , 2015 , 3, 21940-21945	13	13
408	Self-regulation mechanism for charged point defects in hybrid halide perovskites. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 1791-4	16.4	394
407	Stable interface structures of heterovalent semiconductor superlattices: The case of (GaSb) (ZnTe). <i>Computational Materials Science</i> , 2015 , 98, 340-344	3.2	5
406	Impact of bulk properties and local secondary phases on the Cu ₂ (Zn,Sn)Se ₄ solar cells open-circuit voltage. <i>Solar Energy Materials and Solar Cells</i> , 2015 , 133, 119-125	6.4	59
405	Halide perovskite materials for solar cells: a theoretical review. <i>Journal of Materials Chemistry A</i> , 2015 , 3, 8926-8942	13	882
404	Alloy Engineering of Defect Properties in Semiconductors: Suppression of Deep Levels in Transition-Metal Dichalcogenides. <i>Physical Review Letters</i> , 2015 , 115, 126806	7.4	61

403	Origin of and tuning the optical and fundamental band gaps in transparent conducting oxides: The case of M_2O_3 ($M=Al, Ga, In$). <i>Physical Review B</i> , 2015 , 92,	3.3	13
402	H-stabilized shallow acceptors in N-doped ZnO. <i>Physical Review B</i> , 2015 , 92,	3.3	17
401	The origin of electronic band structure anomaly in topological crystalline insulator group-IV tellurides. <i>Npj Computational Materials</i> , 2015 , 1,	10.9	25
400	Surface stability and the selection rules of substrate orientation for optimal growth of epitaxial II-VI semiconductors. <i>Applied Physics Letters</i> , 2015 , 107, 141607	3.4	4
399	Self-regulation of charged defect compensation and formation energy pinning in semiconductors. <i>Scientific Reports</i> , 2015 , 5, 16977	4.9	33
398	Engineering Solar Cell Absorbers by Exploring the Band Alignment and Defect Disparity: The Case of Cu- and Ag-Based Kesterite Compounds. <i>Advanced Functional Materials</i> , 2015 , 25, 6733-6743	15.6	218
397	Tunable Polarity Behavior and Self-Driven Photoswitching in p-WSe ₂ /n-WS ₂ Heterojunctions. <i>Small</i> , 2015 , 11, 5430-8	11	84
396	Highly stable two-dimensional silicon phosphides: Different stoichiometries and exotic electronic properties. <i>Physical Review B</i> , 2015 , 91,	3.3	41
395	Period-doubling reconstructions of semiconductor partial dislocations. <i>NPG Asia Materials</i> , 2015 , 7, e21616	6.2	16
394	Self-Regulation Mechanism for Charged Point Defects in Hybrid Halide Perovskites. <i>Angewandte Chemie</i> , 2015 , 127, 1811-1814	3.6	87
393	Layer-dependent electrical and optoelectronic responses of ReSe ₂ nanosheet transistors. <i>Nanoscale</i> , 2014 , 6, 7226-31	7.7	170
392	Anomalous Alloy Properties in Mixed Halide Perovskites. <i>Journal of Physical Chemistry Letters</i> , 2014 , 5, 3625-31	6.4	188
391	Novel and Enhanced Optoelectronic Performances of Multilayer MoS ₂ /WS ₂ Heterostructure Transistors. <i>Advanced Functional Materials</i> , 2014 , 24, 7025-7031	15.6	320
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4	Revisiting the defect physics in CuInSe/sub 2/ and CuGaSe/sub 2/		3
3	Electronic structure and doping of p-type transparent conducting oxides		1
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1	Comment on [Wide-Range-Tunable p-Type Conductivity of Transparent Cu _{1-x} Br _x Alloy]	15.6	1