

Wan-Jian Yin

List of Publications by Year in descending order

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124
papers

13,398
citations

38742

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21540

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all docs

128
docs citations

128
times ranked

15185
citing authors

#	ARTICLE	IF	CITATIONS
1	Going Beyond the dâ€Band Center to Describe CO ₂ Activation on Single-Atom Alloys. <i>Advanced Energy and Sustainability Research</i> , 2022, 3, 2100152.	5.8	16
2	Effect of alloying on the carrier dynamics in high-performance perovskite solar cells. <i>Journal of Energy Chemistry</i> , 2022, 68, 267-274.	12.9	2
3	Atomistic origin of lattice softness and its impact on structural and carrier dynamics in three dimensional perovskites. <i>Energy and Environmental Science</i> , 2022, 15, 660-671.	30.8	24
4	Interpretation of Rubidium-Based Perovskite Recipes toward Electronic Passivation and Ion-Diffusion Mitigation. <i>Advanced Materials</i> , 2022, 34, e2109998.	21.0	29
5	CsPbI ₃ -Based Phase-Stable 2D Ruddlesden-Popper Perovskites for Efficient Solar Cells. <i>Nano Letters</i> , 2022, 22, 2874-2880.	9.1	22
6	Crystal structure prediction by combining graph network and optimization algorithm. <i>Nature Communications</i> , 2022, 13, 1492.	12.8	26
7	Unique Photoelectric Properties and Defect Tolerance of Lead-Free Perovskite Cs ₃ Cu ₂ I ₅ with Highly Efficient Blue Emission. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 4177-4183.	4.6	12
8	Revisiting the Iodine Vacancy Surface Defects to Rationalize Passivation Strategies in Perovskite Solar Cells. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 6694-6700.	4.6	15
9	High-throughput computational screening of oxide double perovskites for optoelectronic and photocatalysis applications. <i>Journal of Energy Chemistry</i> , 2021, 57, 351-358.	12.9	17
10	High-Performance Blue Perovskite Light-Emitting Diodes Enabled by Efficient Energy Transfer between Coupled Quasi-2D Perovskite Layers. <i>Advanced Materials</i> , 2021, 33, e2005570.	21.0	171
11	Visible-Light Photocatalytic CO ₂ Reduction Using Metal-Organic Framework Derived Ni(OH) ₂ Nanocages: A Synergy from Multiple Light Reflection, Static Charge Transfer, and Oxygen Vacancies. <i>ACS Catalysis</i> , 2021, 11, 345-354.	11.2	117
12	Defect mitigation using <i>scpd</i> -penicillamine for efficient methylammonium-free perovskite solar cells with high operational stability. <i>Chemical Science</i> , 2021, 12, 2050-2059.	7.4	88
13	Strategic synthesis of sponge-like structured SiO _x @CoO multifunctional composites for high-performance and stable lithium-ion batteries. <i>Journal of Materials Chemistry A</i> , 2021, 9, 18440-18453.	10.3	22
14	Atomic-scale insight into the enhanced surface stability of methylammonium lead iodide perovskite by controlled deposition of lead chloride. <i>Energy and Environmental Science</i> , 2021, 14, 4541-4554.	30.8	31
15	Atomistic Mechanism of Passivation of Halide Vacancies in Lead Halide Perovskites by Alkali Ions. <i>Chemistry of Materials</i> , 2021, 33, 1285-1292.	6.7	26
16	Defect states and passivation mechanism at grain boundaries of zinc-blende semiconductors. <i>Semiconductor Science and Technology</i> , 2021, 36, 045028.	2.0	2
17	Multiple-Noncovalent-Interaction-Stabilized Layered Dion-Jacobson Perovskite for Efficient Solar Cells. <i>Nano Letters</i> , 2021, 21, 5788-5797.	9.1	59
18	Density functional theory-free descriptor for the practical discovery of perovskite catalysts. <i>Computational Materials Science</i> , 2021, 193, 110342.	3.0	2

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19	A chalcogenide-cluster-based semiconducting nanotube array with oriented photoconductive behavior. <i>Nature Communications</i> , 2021, 12, 4275.	12.8	17
20	Photoinduced Dynamic Defects Responsible for the Giant, Reversible, and Bidirectional Light-Soaking Effect in Perovskite Solar Cells. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 9328-9335.	4.6	13
21	Significant phonon anharmonicity drives phase transitions in CsPbI ₃ . <i>Applied Physics Letters</i> , 2021, 119, .	3.3	9
22	Flat and Stretched Delafossite $\hat{\pm}$ -AgGaO ₂ : Manipulating Redox Chemistry under Visible Light. <i>ACS Catalysis</i> , 2021, 11, 15083-15088.	11.2	16
23	Designing solar-cell absorber materials through computational high-throughput screening*. <i>Chinese Physics B</i> , 2020, 29, 028803.	1.4	6
24	Passivating Detrimental DX Centers in CH ₃ NH ₃ PbI ₃ for Reducing Nonradiative Recombination and Elongating Carrier Lifetime. <i>Advanced Materials</i> , 2020, 32, e1906115.	21.0	53
25	Simultaneous Low-Order Phase Suppression and Defect Passivation for Efficient and Stable Blue Light-Emitting Diodes. <i>ACS Energy Letters</i> , 2020, 5, 2569-2579.	17.4	89
26	Simple descriptor derived from symbolic regression accelerating the discovery of new perovskite catalysts. <i>Nature Communications</i> , 2020, 11, 3513.	12.8	184
27	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.	5.5	22
28	High Phase Stability in CsPbI ₃ Enabled by Pb ^{II} Octahedra Anchors for Efficient Inorganic Perovskite Photovoltaics. <i>Advanced Materials</i> , 2020, 32, e2000186.	21.0	90
29	Double perovskite Ba ₂ BiTaO ₆ as a promising <i>p</i> -type transparent conductive oxide: A first-principles defect study. <i>Journal of Applied Physics</i> , 2020, 127, .	2.5	7
30	Design of Multifunctional Quinary Metal-Halide Perovskite Compounds Based on Cation ⁺ Anion Co-Ordering. <i>Chemistry of Materials</i> , 2020, 32, 5949-5957.	6.7	10
31	Hexagonal Stacking Faults Act as Hole-Blocking Layers in Lead Halide Perovskites. <i>ACS Energy Letters</i> , 2020, 5, 2231-2233.	17.4	12
32	Bayesian optimization based on a unified figure of merit for accelerated materials screening: A case study of halide perovskites. <i>Science China Materials</i> , 2020, 63, 1024-1035.	6.3	25
33	Coordination assembly of 2D ordered organic metal chalcogenides with widely tunable electronic band gaps. <i>Nature Communications</i> , 2020, 11, 261.	12.8	52
34	Machine learning in materials design: Algorithm and application*. <i>Chinese Physics B</i> , 2020, 29, 116103.	1.4	24
35	Comprehensive first-principles studies on phase stability of copper-based halide perovskite derivatives A _x Cu _m X _n (A = Rb and Cs; X = Cl, Br, and I). <i>Journal of Semiconductors</i> , 2020, 41, 052201.	3.7	11
36	Recent Progress in Defect Tolerance and Defect Passivation in Halide Perovskite Solar Cells. <i>Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica</i> , 2020, .	4.9	9

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37	Computational Modeling and the Design of Perovskite Solar Cells. , 2020, , 2849-2864.		0
38	Theoretical and computational study on defects of solar cell materials. Wuli Xuebao/Acta Physica Sinica, 2020, 69, 177101.	0.5	3
39	Oxide perovskites, double perovskites and derivatives for electrocatalysis, photocatalysis, and photovoltaics. Energy and Environmental Science, 2019, 12, 442-462.	30.8	433
40	Single-phase alkylammonium cesium lead iodide quasi-2D perovskites for color-tunable and spectrum-stable red LEDs. Nanoscale, 2019, 11, 16907-16918.	5.6	24
41	Octahedral gold-silver nanoframes with rich crystalline defects for efficient methanol oxidation manifesting a CO-promoting effect. Nature Communications, 2019, 10, 3782.	12.8	113
42	Plasmon-Free Surface-Enhanced Raman Spectroscopy Using Metallic 2D Materials. ACS Nano, 2019, 13, 8312-8319.	14.6	94
43	Disparity of the Nature of the Band Gap between Halide and Chalcogenide Single Perovskites for Solar Cell Absorbers. Journal of Physical Chemistry Letters, 2019, 10, 4566-4570.	4.6	16
44	Confining MOF-derived SnSe nanoplatelets in nitrogen-doped graphene cages via direct CVD for durable sodium ion storage. Nano Research, 2019, 12, 3051-3058.	10.4	70
45	Achieving High-Quality Sn-Pb Perovskite Films on Complementary Metal-Oxide-Semiconductor-Compatible Metal/Silicon Substrates for Efficient Imaging Array. ACS Nano, 2019, 13, 11800-11808.	14.6	40
46	Materials Design of Solar Cell Absorbers Beyond Perovskites and Conventional Semiconductors via Combining Tetrahedral and Octahedral Coordination. Advanced Materials, 2019, 31, e1806593.	21.0	48
47	Thermodynamic Stability Landscape of Halide Double Perovskites via High-Throughput Computing and Machine Learning. Advanced Functional Materials, 2019, 29, 1807280.	14.9	131
48	Do Chalcogenide Double Perovskites Work as Solar Cell Absorbers: A First-Principles Study. Chemistry of Materials, 2019, 31, 244-250.	6.7	33
49	Computational Modeling and the Design of Perovskite Solar Cells. , 2019, , 1-16.		2
50	Bandgap Engineering of Stable Lead-Free Oxide Double Perovskites for Photovoltaics. Advanced Materials, 2018, 30, e1705901.	21.0	57
51	Solution-Processed Nb-Substituted BaBiO ₃ Double Perovskite Thin Films for Photoelectrochemical Water Reduction. Chemistry of Materials, 2018, 30, 1017-1031.	6.7	45
52	Low-Bandgap Methylammonium-Rubidium Cation Sn-Rich Perovskites for Efficient Ultraviolet-Visible-Near Infrared Photodetectors. Advanced Functional Materials, 2018, 28, 1706068.	14.9	70
53	Intrinsic Point Defects in Inorganic Cesium Lead Iodide Perovskite CsPbI ₃ . Journal of Physical Chemistry C, 2018, 122, 1345-1350.	3.1	144
54	Nanostructured Bi ₂ S ₃ encapsulated within three-dimensional N-doped graphene as active and flexible anodes for sodium-ion batteries. Nano Research, 2018, 11, 4614-4626.	10.4	92

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55	Single Cr atom catalytic growth of graphene. <i>Nano Research</i> , 2018, 11, 2405-2411.	10.4	41
56	Rationalizing Perovskite Data for Machine Learning and Materials Design. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 6948-6954.	4.6	68
57	High-throughput screening of chalcogenide single perovskites by first-principles calculations for photovoltaics. <i>Journal Physics D: Applied Physics</i> , 2018, 51, 474003.	2.8	50
58	Improving the stability and performance of perovskite solar cells <i>via</i> off-the-shelf post-device ligand treatment. <i>Energy and Environmental Science</i> , 2018, 11, 2253-2262.	30.8	181
59	Recent progress in Pb-free stable inorganic double halide perovskites. <i>Journal of Semiconductors</i> , 2018, 39, 071003.	3.7	14
60	Stability Trend of Tilted Perovskites. <i>Journal of Physical Chemistry C</i> , 2018, 122, 15214-15219.	3.1	30
61	Cs ₂ AgBiBr ₆ single-crystal X-ray detectors with a low detection limit. <i>Nature Photonics</i> , 2017, 11, 726-732.	31.4	984
62	Thermodynamic Stability Trend of Cubic Perovskites. <i>Journal of the American Chemical Society</i> , 2017, 139, 14905-14908.	13.7	227
63	Exploring Emerging Photovoltaic Materials Beyond Perovskite: The Case of Skutterudite. <i>Chemistry of Materials</i> , 2017, 29, 9429-9435.	6.7	16
64	Self-compensation in arsenic doping of CdTe. <i>Scientific Reports</i> , 2017, 7, 4563.	3.3	59
65	In Situ Electron Driven Carbon Nanopillar-Fullerene Transformation through Cr Atom Mediation. <i>Nano Letters</i> , 2017, 17, 4725-4732.	9.1	13
66	First-principles study of roles of Cu and Cl in polycrystalline CdTe. <i>Journal of Applied Physics</i> , 2016, 119, .	2.5	44
67	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.	10.3	74
68	Defect Physics of CH ₃ NH ₃ PbX ₃ (X=I, Br, Cl) Perovskites. , 2016, , 79-105.		19
69	Orbital-frustration-induced ordering in semiconductor alloys. <i>Physical Review B</i> , 2016, 93, .	3.2	1
70	Review on first-principles study of defect properties of CdTe as a solar cell absorber. <i>Semiconductor Science and Technology</i> , 2016, 31, 083002.	2.0	109
71	Two-Dimensional SiS Layers with Promising Electronic and Optoelectronic Properties: Theoretical Prediction. <i>Nano Letters</i> , 2016, 16, 1110-1117.	9.1	149
72	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.	3.3	5

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73	Self-regulation of charged defect compensation and formation energy pinning in semiconductors. Scientific Reports, 2015, 5, 16977.	3.3	56
74	Physics of grain boundaries in polycrystalline photovoltaic semiconductors. Journal of Applied Physics, 2015, 117, .	2.5	52
75	Superior Photovoltaic Properties of Lead Halide Perovskites: Insights from First-Principles Theory. Journal of Physical Chemistry C, 2015, 119, 5253-5264.	3.1	246
76	Device Performance of the Mott Insulator LaVO_3 as a Photovoltaic Material. Physical Review Applied, 2015, 3, .	3.8	73
77	Unipolar self-doping behavior in perovskite $\text{CH}_3\text{NH}_3\text{PbBr}_3$. Applied Physics Letters, 2015, 106, .	3.3	181
78	Origin of High Electronic Quality in Structurally Disordered $\text{CH}_3\text{NH}_3\text{PbI}_3$ and the Passivation Effect of Cl and O at Grain Boundaries. Advanced Electronic Materials, 2015, 1, 1500044.	5.1	175
79	Theoretical and experimental study of earth-abundant solar cell materials. , 2015, , .		0
80	Enhanced p-type dopability of P and As in CdTe using non-equilibrium thermal processing. Journal of Applied Physics, 2015, 118, .	2.5	60
81	Monitoring the stability of organometallic perovskite thin films. Journal of Materials Chemistry A, 2015, 3, 21940-21945.	10.3	13
82	LDA+U/GGA+U calculations of structural and electronic properties of CdTe: Dependence on the effective U parameter. Computational Materials Science, 2015, 98, 18-23.	3.0	25
83	Halide perovskite materials for solar cells: a theoretical review. Journal of Materials Chemistry A, 2015, 3, 8926-8942.	10.3	1,114
84	Defect Physics in Photovoltaic Materials Revealed by Combined High-Resolution Microscopy and Density-Functional Theory Calculation. Microscopy and Microanalysis, 2014, 20, 514-515.	0.4	1
85	Creating intermediate bands in ZnTe via co-alloying approach. Applied Physics Express, 2014, 7, 121201.	2.4	7
86	Determination of Polarization Fields Across Polytype Interfaces in InAs Nanopillars. Advanced Materials, 2014, 26, 1052-1057.	21.0	27
87	Engineering Grain Boundaries in $\text{Cu}_2\text{ZnSnSe}_4$ for Better Cell Performance: A First-Principle Study. Advanced Energy Materials, 2014, 4, 1300712.	19.5	135
88	Unusual defect physics in $\text{CH}_3\text{NH}_3\text{PbI}_3$ perovskite solar cell absorber. Applied Physics Letters, 2014, 104, .	3.3	2,142
89	Grain-Boundary-Enhanced Carrier Collection in CdTe Solar Cells. Physical Review Letters, 2014, 112, 156103.	7.8	258
90	Unique Properties of Halide Perovskites as Possible Origins of the Superior Solar Cell Performance. Advanced Materials, 2014, 26, 4653-4658.	21.0	1,735

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91	Predictions for p-Type $\text{CH}_3\text{NH}_3\text{PbI}_3$ Perovskites. Journal of Physical Chemistry C, 2014, 118, 25350-25354.	3.1	71
92	Anomalous Alloy Properties in Mixed Halide Perovskites. Journal of Physical Chemistry Letters, 2014, 5, 3625-3631.	4.6	231
93	Stability, transparency, and conductivity of $\text{Mg}_x\text{Zn}_{1-x}\text{O}$ and $\text{Cd}_x\text{Zn}_{1-x}\text{O}$: Designing optimum transparency conductive oxides. Journal of Applied Physics, 2014, 115, .	2.5	10
94	Carrier Separation at Dislocation Pairs in CdTe. Physical Review Letters, 2013, 111, 096403.	7.8	51
95	Structural, electronic, and optical properties of Cu_3VVI_4 compound semiconductors. Applied Physics Letters, 2013, 103, .	3.3	36
96	From atomic structure to photovoltaic properties in CdTe solar cells. Ultramicroscopy, 2013, 134, 113-125.	1.9	80
97	Control of one-dimensional magnetism in graphene via spontaneous hydrogenation of the grain boundary. Physical Chemistry Chemical Physics, 2013, 15, 8271.	2.8	5
98	The structure and properties of (aluminum, oxygen) defect complexes in silicon. Journal of Applied Physics, 2013, 114, 063520.	2.5	10
99	Defect segregation at grain boundary and its impact on photovoltaic performance of CuInSe_2 . Applied Physics Letters, 2013, 102, .	3.3	50
100	The electronic properties of point defects in earth-abundant photovoltaic material Zn_3P_2 : A hybrid functional method study. Journal of Applied Physics, 2013, 113, .	2.5	26
101	First principles study of aluminum-oxygen complexes in silicon. , 2013, , .		0
102	Electrostatic Potentials at $\text{Cu}(\text{In,Ga})\text{Se}_2$ Grain Boundaries: Experiment and Simulations. Physical Review Letters, 2012, 109, 095506.	7.8	39
103	Electronic and optical properties of $\text{Co}_x\text{Al}_{1-x}\text{Ga}_{1-x}\text{In}_x$ alloys. Applied Physics Letters, 2012, 100, .	3.3	15
104	Comparative study of defect transition energy calculation methods: The case of oxygen vacancy in In_2O_3 . Physical Review B, 2012, 86, .	3.2	23
105	Possible effects of oxygen in Te-rich $\text{Fe}_3(112)$ grain boundaries in CdTe. Solid State Communications, 2012, 152, 1744-1747.	1.9	27
106	Strong asymmetrical doping properties of spinel CoAl_2O_4 . Journal of Applied Physics, 2012, 111, 093723.	2.5	6
107	Realizing a SnO_2 -based ultraviolet light-emitting diode via breaking the dipole-forbidden rule. NPC Asia Materials, 2012, 4, e30-e30.	7.9	137
108	Titanium and magnesium Co-alloyed hematite thin films for photoelectrochemical water splitting. Journal of Applied Physics, 2012, 111, 073502.	2.5	30

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109	Origin of the diverse behavior of oxygen vacancies in ABO ₃ perovskites: A symmetry based analysis. Physical Review B, 2012, 85, .	3.2	28
110	A Novel Codoping Approach for Enhancing the Performance of LiFePO ₄ Cathodes. Advanced Energy Materials, 2012, 2, 1028-1032.	19.5	72
111	Polarization-Induced Charge Distribution at Homogeneous Zincblende/Wurtzite Heterostructural Junctions in ZnSe Nanobelts. Advanced Materials, 2012, 24, 1328-1332.	21.0	30
112	Double-Hole-Mediated Coupling of Dopants and Its Impact on Band Gap Engineering in TiO_2 . Physical Review Letters, 2011, 106, 066801.	7.8	134
113	Doping properties of monoclinic BiVO ₄ studied by first-principles density-functional theory. Physical Review B, 2011, 83, .	3.2	194
114	Origin of Bonding between the SWCNT and the Fe ₃ O ₄ (001) Surface and the Enhanced Electrical Conductivity. Journal of Physical Chemistry Letters, 2011, 2, 2853-2858.	4.6	17
115	Prediction of the chemical trends of oxygen vacancy levels in binary metal oxides. Applied Physics Letters, 2011, 99, .	3.3	42
116	Effective band gap narrowing of anatase TiO ₂ by strain along a soft crystal direction. Applied Physics Letters, 2010, 96, .	3.3	185
117	Band structure engineering of semiconductors for enhanced photoelectrochemical water splitting: The case of TiO_2 . Physical Review B, 2010, 82, .	3.2	300
118	Revised <i>ab initio</i> natural band offsets of all group IV, II-VI, and III-V semiconductors. Applied Physics Letters, 2009, 94, .	3.3	188
119	Hybridized kinetic energy functional for orbital-free density functional method. Physics Letters, Section A: General, Atomic and Solid State Physics, 2009, 373, 480-483.	2.1	1
120	Electronic structure and phase stability of MgTe, ZnTe, CdTe, and their alloys in the B_3 , B_4 , and B_8 structures. Physical Review B, 2009, 79, .	3.2	55
121	Quaternary semiconductors with positive crystal field splitting: Potential high-efficiency spin-polarized electron sources. Applied Physics Letters, 2009, 95, .	3.3	14
122	Magic number 32 and 90 of metal clusters: A shell jellium model study. Solid State Communications, 2008, 147, 323-326.	1.9	11
123	Origin of the unusually large band-gap bowing and the breakdown of the band-edge distribution rule in the $\text{Sn}_x\text{Ge}_{1-x}$ alloys. Physical Review B, 2008, 78, .	3.2	149
124	Defect calculations with quasiparticle correction: A revisited study of iodine defects in CH ₃ NH ₃ PbI ₃ . Chinese Physics B, 0, , .	1.4	0