Wan-Jian Yin

List of Publications by Year
in descending order

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124 papers	13,398 citations	38742 50 h-index	21540 114 g-index
128 all docs	128 docs citations	128 times ranked	15185 citing authors

#	Article	IF	Citations
1	Unusual defect physics in CH3NH3PbI3 perovskite solar cell absorber. Applied Physics Letters, 2014, 104, .	3.3	2,142
2	Unique Properties of Halide Perovskites as Possible Origins of the Superior Solar Cell Performance. Advanced Materials, 2014, 26, 4653-4658.	21.0	1,735
3	Halide perovskite materials for solar cells: a theoretical review. Journal of Materials Chemistry A, 2015, 3, 8926-8942.	10.3	1,114
4	Cs2AgBiBr6 single-crystal X-ray detectors with a low detection limit. Nature Photonics, 2017, 11, 726-732.	31.4	984
5	Oxide perovskites, double perovskites and derivatives for electrocatalysis, photocatalysis, and photovoltaics. Energy and Environmental Science, 2019, 12, 442-462.	30.8	433
6	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, .	3.2	300
7	Grain-Boundary-Enhanced Carrier Collection in CdTe Solar Cells. Physical Review Letters, 2014, 112, 156103.	7.8	258
8	Superior Photovoltaic Properties of Lead Halide Perovskites: Insights from First-Principles Theory. Journal of Physical Chemistry C, 2015, 119, 5253-5264.	3.1	246
9	Anomalous Alloy Properties in Mixed Halide Perovskites. Journal of Physical Chemistry Letters, 2014, 5, 3625-3631.	4.6	231
10	Thermodynamic Stability Trend of Cubic Perovskites. Journal of the American Chemical Society, 2017, 139, 14905-14908.	13.7	227
11	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, .	3.2	194
12	Revised ab initio natural band offsets of all group IV, II-VI, and III-V semiconductors. Applied Physics Letters, 2009, 94, .	3.3	188
13	Effective band gap narrowing of anatase TiO2 by strain along a soft crystal direction. Applied Physics Letters, 2010, 96, .	3.3	185
14	Simple descriptor derived from symbolic regression accelerating the discovery of new perovskite catalysts. Nature Communications, 2020, 11, 3513.	12.8	184
15	Unipolar self-doping behavior in perovskite CH3NH3PbBr3. Applied Physics Letters, 2015, 106, .	3.3	181
16	Improving the stability and performance of perovskite solar cells via off-the-shelf post-device ligand treatment. Energy and Environmental Science, 2018, 11, 2253-2262.	30.8	181
17	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.	5.1	175
18	Highâ€Performance Blue Perovskite Lightâ€Emitting Diodes Enabled by Efficient Energy Transfer between Coupled Quasiâ€2D Perovskite Layers. Advanced Materials, 2021, 33, e2005570.	21.0	171

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19	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, .	3.2	149
20	Two-Dimensional SiS Layers with Promising Electronic and Optoelectronic Properties: Theoretical Prediction. Nano Letters, 2016, 16, 1110-1117.	9.1	149
21	Intrinsic Point Defects in Inorganic Cesium Lead Iodide Perovskite CsPbI₃. Journal of Physical Chemistry C, 2018, 122, 1345-1350.	3.1	144
22	Realizing a SnO2-based ultraviolet light-emitting diode via breaking the dipole-forbidden rule. NPG Asia Materials, 2012, 4, e30-e30.	7.9	137
23	Engineering Grain Boundaries in Cu₂ZnSnSe₄ for Better Cell Performance: A Firstâ€Principle Study. Advanced Energy Materials, 2014, 4, 1300712.	19.5	135
24	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.	7.8	134
25	Thermodynamic Stability Landscape of Halide Double Perovskites via Highâ€Throughput Computing and Machine Learning. Advanced Functional Materials, 2019, 29, 1807280.	14.9	131
26	Visible-Light Photocatalytic CO₂ Reduction Using Metal-Organic Framework Derived Ni(OH)₂ Nanocages: A Synergy from Multiple Light Reflection, Static Charge Transfer, and Oxygen Vacancies. ACS Catalysis, 2021, 11, 345-354.	11.2	117
27	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
28	Review on first-principles study of defect properties of CdTe as a solar cell absorber. Semiconductor Science and Technology, 2016, 31, 083002.	2.0	109
29	Plasmon-Free Surface-Enhanced Raman Spectroscopy Using Metallic 2D Materials. ACS Nano, 2019, 13, 8312-8319.	14.6	94
30	Nanostructured Bi2S3 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
31	High Phase Stability in CsPbI₃ Enabled by Pbâ€"I Octahedra Anchors for Efficient Inorganic Perovskite Photovoltaics. Advanced Materials, 2020, 32, e2000186.	21.0	90
32	Simultaneous Low-Order Phase Suppression and Defect Passivation for Efficient and Stable Blue Light-Emitting Diodes. ACS Energy Letters, 2020, 5, 2569-2579.	17.4	89
33	Defect mitigation using <scp>d</scp>-penicillamine for efficient methylammonium-free perovskite solar cells with high operational stability. Chemical Science, 2021, 12, 2050-2059.	7.4	88
34	From atomic structure to photovoltaic properties in CdTe solar cells. Ultramicroscopy, 2013, 134, 113-125.	1.9	80
35	Fast self-diffusion of ions in CH₃NH₃PbI₃: the interstiticaly mechanism versus vacancy-assisted mechanism. Journal of Materials Chemistry A, 2016, 4, 13105-13112.	10.3	74
36	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></mml:mrow></mml:msub></mml:mrow></mml:math> a Photovoltaic Material. Physical Review Applied, 2015, 3, .	3.8	73

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37	A Novel Codoping Approach for Enhancing the Performance of LiFePO₄ Cathodes. Advanced Energy Materials, 2012, 2, 1028-1032.	19.5	72
38	Predictions for p-Type CH₃NH₃PbI₃ Perovskites. Journal of Physical Chemistry C, 2014, 118, 25350-25354.	3.1	71
39	Lowâ€Bandgap Methylammoniumâ€Rubidium Cation Snâ€Rich Perovskites for Efficient Ultravioletâ€“Visibleâ€“Near Infrared Photodetectors. Advanced Functional Materials, 2018, 28, 1706068.	14.9	70
40	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
41	Rationalizing Perovskite Data for Machine Learning and Materials Design. Journal of Physical Chemistry Letters, 2018, 9, 6948-6954.	4.6	68
42	Enhanced p-type dopability of P and As in CdTe using non-equilibrium thermal processing. Journal of Applied Physics, 2015, 118, .	2.5	60
43	Self-compensation in arsenic doping of CdTe. Scientific Reports, 2017, 7, 4563.	3.3	59
44	Multiple-Noncovalent-Interaction-Stabilized Layered Dionâ€“Jacobson Perovskite for Efficient Solar Cells. Nano Letters, 2021, 21, 5788-5797.	9.1	59
45	Bandgap Engineering of Stable Leadâ€Free Oxide Double Perovskites for Photovoltaics. Advanced Materials, 2018, 30, e1705901.	21.0	57
46	Self-regulation of charged defect compensation and formation energy pinning in semiconductors. Scientific Reports, 2015, 5, 16977.	3.3	56
47	Electronic structure and phase stability of MgTe, ZnTe, CdTe, and their alloys in theB3,B4, andB8 structures. Physical Review B, 2009, 79, .	3.2	55
48	Passivating Detrimental DX Centers in CH₃NH₃PbI₃ for Reducing Nonradiative Recombination and Elongating Carrier Lifetime. Advanced Materials, 2020, 32, e1906115.	21.0	53
49	Physics of grain boundaries in polycrystalline photovoltaic semiconductors. Journal of Applied Physics, 2015, 117, .	2.5	52
50	Coordination assembly of 2D ordered organic metal chalcogenides with widely tunable electronic band gaps. Nature Communications, 2020, 11, 261.	12.8	52
51	Carrier Separation at Dislocation Pairs in CdTe. Physical Review Letters, 2013, 111, 096403.	7.8	51
52	Defect segregation at grain boundary and its impact on photovoltaic performance of CuInSe2. Applied Physics Letters, 2013, 102, .	3.3	50
53	High-throughput screening of chalcogenide single perovskites by first-principles calculations for photovoltaics. Journal Physics D: Applied Physics, 2018, 51, 474003.	2.8	50
54	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

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55	Solution-Processed Nb-Substituted BaBiO₃ Double Perovskite Thin Films for Photoelectrochemical Water Reduction. Chemistry of Materials, 2018, 30, 1017-1031.	6.7	45
56	First-principles study of roles of Cu and Cl in polycrystalline CdTe. Journal of Applied Physics, 2016, 119, .	2.5	44
57	Prediction of the chemical trends of oxygen vacancy levels in binary metal oxides. Applied Physics Letters, 2011, 99, .	3.3	42
58	Single Cr atom catalytic growth of graphene. Nano Research, 2018, 11, 2405-2411.	10.4	41
59	Achieving High-Quality Snâ€“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
60	Electrostatic Potentials at Cu(In,Ga)<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Se</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>Grain Boundaries: Experiment and Simulations. Physical Review Letters, 2012, 109, 095506.	7.8	39
61	Structural, electronic, and optical properties of Cu3-V-VI4 compound semiconductors. Applied Physics Letters, 2013, 103, .	3.3	36
62	Do Chalcogenide Double Perovskites Work as Solar Cell Absorbers: A First-Principles Study. Chemistry of Materials, 2019, 31, 244-250.	6.7	33
63	Atomic-scale insight into the enhanced surface stability of methylammonium lead iodide perovskite by controlled deposition of lead chloride. Energy and Environmental Science, 2021, 14, 4541-4554.	30.8	31
64	Titanium and magnesium Co-alloyed hematite thin films for photoelectrochemical water splitting. Journal of Applied Physics, 2012, 111, 073502.	2.5	30
65	Polarizationâ€Induced Charge Distribution at Homogeneous Zincblende/Wurtzite Heterostructural Junctions in ZnSe Nanobelts. Advanced Materials, 2012, 24, 1328-1332.	21.0	30
66	Stability Trend of Tilted Perovskites. Journal of Physical Chemistry C, 2018, 122, 15214-15219.	3.1	30
67	Interpretation of Rubidiumâ€Based Perovskite Recipes toward Electronic Passivation and Ionâ€Diffusion Mitigation. Advanced Materials, 2022, 34, e2109998.	21.0	29
68	Origin of the diverse behavior of oxygen vacancies inABO3perovskites: A symmetry based analysis. Physical Review B, 2012, 85, .	3.2	28
69	Possible effects of oxygen in Te-rich Î£3 (112) grain boundaries in CdTe. Solid State Communications, 2012, 152, 1744-1747.	1.9	27
70	Determination of Polarizationâ€Fields Across Polytype Interfaces in InAs Nanopillars. Advanced Materials, 2014, 26, 1052-1057.	21.0	27
71	The electronic properties of point defects in earth-abundant photovoltaic material Zn3P2: A hybrid functional method study. Journal of Applied Physics, 2013, 113, .	2.5	26
72	Atomistic Mechanism of Passivation of Halide Vacancies in Lead Halide Perovskites by Alkali Ions. Chemistry of Materials, 2021, 33, 1285-1292.	6.7	26

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73	Crystal structure prediction by combining graph network and optimization algorithm. Nature Communications, 2022, 13, 1492.	12.8	26
74	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
75	Bayesian optimization based on a unified figure of merit for accelerated materials screening: A case study of halide perovskites. Science China Materials, 2020, 63, 1024-1035.	6.3	25
76	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
77	Machine learning in materials design: Algorithm and application*. Chinese Physics B, 2020, 29, 116103.	1.4	24
78	Atomistic origin of lattice softness and its impact on structural and carrier dynamics in three dimensional perovskites. Energy and Environmental Science, 2022, 15, 660-671.	30.8	24
79	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, .	3.2	23
80	Searching for stable perovskite solar cell materials using materials genome techniques and high-throughput calculations. Journal of Materials Chemistry C, 2020, 8, 12012-12035.	5.5	22
81	Strategic synthesis of sponge-like structured SiO_x@C@CoO multifunctional composites for high-performance and stable lithium-ion batteries. Journal of Materials Chemistry A, 2021, 9, 18440-18453.	10.3	22
82	CsPbI₃-Based Phase-Stable 2D Ruddlesdenâ€“Popper Perovskites for Efficient Solar Cells. Nano Letters, 2022, 22, 2874-2880.	9.1	22
83	Defect Physics of CH3NH3PbX3 (XÂ=ÂI, Br, Cl) Perovskites. , 2016, , 79-105.		19
84	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.	4.6	17
85	High-throughput computational screening of oxide double perovskites for optoelectronic and photocatalysis applications. Journal of Energy Chemistry, 2021, 57, 351-358.	12.9	17
86	A chalcogenide-cluster-based semiconducting nanotube array with oriented photoconductive behavior. Nature Communications, 2021, 12, 4275.	12.8	17
87	Exploring Emerging Photovoltaic Materials Beyond Perovskite: The Case of Skutterudite. Chemistry of Materials, 2017, 29, 9429-9435.	6.7	16
88	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
89	Going Beyond the dâ€Band Center to Describe CO₂ Activation on Singleâ€Atom Alloys. Advanced Energy and Sustainability Research, 2022, 3, 2100152.	5.8	16
90	Flat and Stretched Delafossite Î±-AgGaO₂: Manipulating Redox Chemistry under Visible Light. ACS Catalysis, 2021, 11, 15083-15088.	11.2	16

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91	Electronic and optical properties of CoX2O4 (Xâ€‰=â€‰Al, Ga, In) alloys. Applied Physics Letters, 2012, 100, .	3.3	15
92	Revisiting the Iodine Vacancy Surface Defects to Rationalize Passivation Strategies in Perovskite Solar Cells. Journal of Physical Chemistry Letters, 2022, 13, 6694-6700.	4.6	15
93	Quaternary semiconductors with positive crystal field splitting: Potential high-efficiency spin-polarized electron sources. Applied Physics Letters, 2009, 95, .	3.3	14
94	Recent progress in Pb-free stable inorganic double halide perovskites. Journal of Semiconductors, 2018, 39, 071003.	3.7	14
95	Monitoring the stability of organometallic perovskite thin films. Journal of Materials Chemistry A, 2015, 3, 21940-21945.	10.3	13
96	In Situ Electron Driven Carbon Nanopillar-Fullerene Transformation through Cr Atom Mediation. Nano Letters, 2017, 17, 4725-4732.	9.1	13
97	Photoinduced Dynamic Defects Responsible for the Giant, Reversible, and Bidirectional Light-Soaking Effect in Perovskite Solar Cells. Journal of Physical Chemistry Letters, 2021, 12, 9328-9335.	4.6	13
98	Hexagonal Stacking Faults Act as Hole-Blocking Layers in Lead Halide Perovskites. ACS Energy Letters, 2020, 5, 2231-2233.	17.4	12
99	Unique Photoelectric Properties and Defect Tolerance of Lead-Free Perovskite Cs₃Cu₂I₅ with Highly Efficient Blue Emission. Journal of Physical Chemistry Letters, 2022, 13, 4177-4183.	4.6	12
100	Magic number 32 and 90 of metal clusters: A shell jellium model study. Solid State Communications, 2008, 147, 323-326.	1.9	11
101	Comprehensive first-principles studies on phase stability of copper-based halide perovskite derivatives A_lCu_mX_n (A = Rb and Cs; X = Cl, Br, and I). Journal of Semiconductors, 2020, 41, 052201.	3.7	11
102	The structure and properties of (aluminum, oxygen) defect complexes in silicon. Journal of Applied Physics, 2013, 114, 063520.	2.5	10
103	Stability, transparency, and conductivity of MgxZn1â^'xO and CdxZn1â^'xO: Designing optimum transparency conductive oxides. Journal of Applied Physics, 2014, 115, .	2.5	10
104	Design of Multifunctional Quinternary Metal-Halide Perovskite Compounds Based on Cationâ€“Anion Co-Ordering. Chemistry of Materials, 2020, 32, 5949-5957.	6.7	10
105	Recent Progress in Defect Tolerance and Defect Passivation in Halide Perovskite Solar Cells. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2020, .	4.9	9
106	Significant phonon anharmonicity drives phase transitions in CsPbI3. Applied Physics Letters, 2021, 119, .	3.3	9
107	Creating intermediate bands in ZnTe via co-alloying approach. Applied Physics Express, 2014, 7, 121201.	2.4	7
108	Double perovskite Ba2BiTaO6 as a promising p-type transparent conductive oxide: A first-principles defect study. Journal of Applied Physics, 2020, 127, .	2.5	7

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109	Strong asymmetrical doping properties of spinel CoAl2O4. Journal of Applied Physics, 2012, 111, 093723.	2.5	6
110	Designing solar-cell absorber materials through computational high-throughput screening*. Chinese Physics B, 2020, 29, 028803.	1.4	6
111	Control of one-dimensional magnetism in graphene via spontaneous hydrogenation of the grain boundary. Physical Chemistry Chemical Physics, 2013, 15, 8271.	2.8	5
112	Surface stability and the selection rules of substrate orientation for optimal growth of epitaxial II-VI semiconductors. Applied Physics Letters, 2015, 107, 141607.	3.3	5
113	Theoretical and computational study on defects of solar cell materials. Wuli Xuebao/Acta Physica Sinica, 2020, 69, 177101.	0.5	3
114	Defect states and passivation mechanism at grain boundaries of zinc-blende semiconductors. Semiconductor Science and Technology, 2021, 36, 045028.	2.0	2
115	Density functional theory-free descriptor for the practical discovery of perovskite catalysts. Computational Materials Science, 2021, 193, 110342.	3.0	2
116	Computational Modeling and the Design of Perovskite Solar Cells. , 2019, , 1-16.		2
117	Effect of alloying on the carrier dynamics in high-performance perovskite solar cells. Journal of Energy Chemistry, 2022, 68, 267-274.	12.9	2
118	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
119	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
120	Orbital-frustration-induced ordering in semiconductor alloys. Physical Review B, 2016, 93, .	3.2	1
121	First principles study of aluminum-oxygen complexes in silicon. , 2013, , .		0
122	Theoretical and experimental study of earth-abundant solar cell materials. , 2015, , .		0
123	Defect calculations with quasiparticle correction: A revisited study of iodine defects in CH3NH3PbI3. Chinese Physics B, 0, , .	1.4	0
124	Computational Modeling and the DesignÂofÂPerovskite Solar Cells. , 2020, , 2849-2864.		0