

## List of Publications by Citations

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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.

158 papers	10,966 citations	52 h-index	102 g-index
169 ext. papers	13,613 ext. citations	10.1 avg, IF	6.6 L-index

#	Paper	IF	Citations
158	Efficient and stable emission of warm-white light from lead-free halide double perovskites. <i>Nature</i> , <b>2018</b> , 563, 541-545	50.4	835
157	Thermodynamically stabilized $\text{ECsPbI}$ -based perovskite solar cells with efficiencies >18. <i>Science</i> , <b>2019</b> , 365, 591-595	33.3	644
156	Density Functional study of FeS, FeSe, and FeTe: Electronic structure, magnetism, phonons, and superconductivity. <i>Physical Review B</i> , <b>2008</b> , 78,	3.3	644
155	Highly Oriented Low-Dimensional Tin Halide Perovskites with Enhanced Stability and Photovoltaic Performance. <i>Journal of the American Chemical Society</i> , <b>2017</b> , 139, 6693-6699	16.4	558
154	Design of Lead-Free Inorganic Halide Perovskites for Solar Cells via Cation-Transmutation. <i>Journal of the American Chemical Society</i> , <b>2017</b> , 139, 2630-2638	16.4	490
153	Doping Lanthanide into Perovskite Nanocrystals: Highly Improved and Expanded Optical Properties. <i>Nano Letters</i> , <b>2017</b> , 17, 8005-8011	11.5	447
152	Ultrasensitive detection of miRNA with an antimonene-based surface plasmon resonance sensor. <i>Nature Communications</i> , <b>2019</b> , 10, 28	17.4	309
151	Strain engineering in perovskite solar cells and its impacts on carrier dynamics. <i>Nature Communications</i> , <b>2019</b> , 10, 815	17.4	286
150	Electronic correlations in the iron pnictides. <i>Nature Physics</i> , <b>2009</b> , 5, 647-650	16.2	285
149	Materials discovery at high pressures. <i>Nature Reviews Materials</i> , <b>2017</b> , 2,	73.3	266
148	Zn-Alloyed CsPbI Nanocrystals for Highly Efficient Perovskite Light-Emitting Devices. <i>Nano Letters</i> , <b>2019</b> , 19, 1552-1559	11.5	256
147	Efficient and stable Ruddlesden-Popper perovskite solar cell with tailored interlayer molecular interaction. <i>Nature Photonics</i> , <b>2020</b> , 14, 154-163	33.9	251
146	Trifluoroacetate induced small-grained CsPbBr perovskite films result in efficient and stable light-emitting devices. <i>Nature Communications</i> , <b>2019</b> , 10, 665	17.4	227
145	Cu-In Halide Perovskite Solar Absorbers. <i>Journal of the American Chemical Society</i> , <b>2017</b> , 139, 6718-6725	16.4	226
144	Atomically engineering activation sites onto metallic 1T-MoS catalysts for enhanced electrochemical hydrogen evolution. <i>Nature Communications</i> , <b>2019</b> , 10, 982	17.4	180
143	Rational Design of Halide Double Perovskites for Optoelectronic Applications. <i>Joule</i> , <b>2018</b> , 2, 1662-1673	27.8	179
142	Chlorine-Incorporation-Induced Formation of the Layered Phase for Antimony-Based Lead-Free Perovskite Solar Cells. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 1019-1027	16.4	178

141	Density functional study of excess Fe in Fe <sub>1+x</sub> Te: Magnetism and doping. <i>Physical Review B</i> , <b>2009</b> , 79,	3.3	149
140	Pressure-induced emission of cesium lead halide perovskite nanocrystals. <i>Nature Communications</i> , <b>2018</b> , 9, 4506	17.4	134
139	Colloidal Synthesis of Ternary Copper Halide Nanocrystals for High-Efficiency Deep-Blue Light-Emitting Diodes with a Half-Lifetime above 100 h. <i>Nano Letters</i> , <b>2020</b> , 20, 3568-3576	11.5	121
138	Fast Diffusion of Native Defects and Impurities in Perovskite Solar Cell Material CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> . <i>Chemistry of Materials</i> , <b>2016</b> , 28, 4349-4357	9.6	112
137	Functionality-Directed Screening of Pb-Free Hybrid Organic/Inorganic Perovskites with Desired Intrinsic Photovoltaic Functionalities. <i>Chemistry of Materials</i> , <b>2017</b> , 29, 524-538	9.6	110
136	Stable Yellow Light-Emitting Devices Based on Ternary Copper Halides with Broadband Emissive Self-Trapped Excitons. <i>ACS Nano</i> , <b>2020</b> , 14, 4475-4486	16.7	106
135	Tellurium Hydrides at High Pressures: High-Temperature Superconductors. <i>Physical Review Letters</i> , <b>2016</b> , 116, 057002	7.4	104
134	CALYPSO structure prediction method and its wide application. <i>Computational Materials Science</i> , <b>2016</b> , 112, 406-415	3.2	102
133	Stabilizing Perovskite Solar Cells to IEC61215:2016 Standards with over 9,000-h Operational Tracking. <i>Joule</i> , <b>2020</b> , 4, 2646-2660	27.8	97
132	CsPb(I Br) <sub>1-x</sub> solar cells. <i>Science Bulletin</i> , <b>2019</b> , 64, 1532-1539	10.6	92
131	Pseudohalide-Induced Recrystallization Engineering for CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> Film and Its Application in Highly Efficient Inverted Planar Heterojunction Perovskite Solar Cells. <i>Advanced Functional Materials</i> , <b>2018</b> , 28, 1704836	15.6	92
130	Electrically-Driven Violet Light-Emitting Devices Based on Highly Stable Lead-Free Perovskite Cs <sub>3</sub> Sb <sub>2</sub> Br <sub>9</sub> Quantum Dots. <i>ACS Energy Letters</i> , <b>2020</b> , 5, 385-394	20.1	90
129	First-principles study of electron-phonon coupling in hole- and electron-doped diamonds in the virtual crystal approximation. <i>Physical Review B</i> , <b>2005</b> , 72,	3.3	89
128	Formation and Diffusion of Metal Impurities in Perovskite Solar Cell Material CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> : Implications on Solar Cell Degradation and Choice of Electrode. <i>Advanced Science</i> , <b>2018</b> , 5, 1700662	13.6	82
127	Robust Stability of Efficient Lead-Free Formamidinium Tin Iodide Perovskite Solar Cells Realized by Structural Regulation. <i>Journal of Physical Chemistry Letters</i> , <b>2018</b> , 9, 6999-7006	6.4	79
126	Perovskite Solar Absorbers: Materials by Design. <i>Small Methods</i> , <b>2018</b> , 2, 1700316	12.8	78
125	InSe: a two-dimensional material with strong interlayer coupling. <i>Nanoscale</i> , <b>2018</b> , 10, 7991-7998	7.7	76
124	Two-Dimensional PC with Direct Band Gap and Anisotropic Carrier Mobility. <i>Journal of the American Chemical Society</i> , <b>2019</b> , 141, 1599-1605	16.4	76

123	High Color-Rendering Index and Stable White Light-Emitting Diodes by Assembling Two Broadband Emissive Self-Trapped Excitons. <i>Advanced Materials</i> , <b>2021</b> , 33, e2001367	24	74
122	A Unified Understanding of the Thickness-Dependent Bandgap Transition in Hexagonal Two-Dimensional Semiconductors. <i>Journal of Physical Chemistry Letters</i> , <b>2016</b> , 7, 597-602	6.4	72
121	Thermochromic Lead-Free Halide Double Perovskites. <i>Advanced Functional Materials</i> , <b>2019</b> , 29, 1807375	15.6	69
120	Intrinsic Defect Properties in Halide Double Perovskites for Optoelectronic Applications. <i>Physical Review Applied</i> , <b>2018</b> , 10,	4.3	69
119	Wide InP nanowires with wurtzite/zincblende superlattice segments are type-II whereas narrower nanowires become type-I: an atomistic pseudopotential calculation. <i>Nano Letters</i> , <b>2010</b> , 10, 4055-60	11.5	68
118	Ba-induced phase segregation and band gap reduction in mixed-halide inorganic perovskite solar cells. <i>Nature Communications</i> , <b>2019</b> , 10, 4686	17.4	65
117	Materials discovery via CALYPSO methodology. <i>Journal of Physics Condensed Matter</i> , <b>2015</b> , 27, 203203	1.8	63
116	Solid salt confinement effect: An effective strategy to fabricate high crystalline polymer carbon nitride for enhanced photocatalytic hydrogen evolution. <i>Applied Catalysis B: Environmental</i> , <b>2019</b> , 246, 349-355	21.8	62
115	Zintl-phase compounds with SnSb <sub>4</sub> tetrahedral anions: Electronic structure and thermoelectric properties. <i>Physical Review B</i> , <b>2010</b> , 81,	3.3	62
114	Stabilization of fullerene-like boron cages by transition metal encapsulation. <i>Nanoscale</i> , <b>2015</b> , 7, 10482-9	7.7	59
113	Nanoporous Sulfur-Doped Copper Oxide (CuOS) for Overall Water Splitting. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2018</b> , 10, 745-752	9.5	59
112	High-Pressure Phase Stability and Superconductivity of Pnictogen Hydrides and Chemical Trends for Compressed Hydrides. <i>Chemistry of Materials</i> , <b>2016</b> , 28, 1746-1755	9.6	57
111	Evolution of electronic structure as a function of layer thickness in group-VIB transition metal dichalcogenides: emergence of localization prototypes. <i>Nano Letters</i> , <b>2015</b> , 15, 949-57	11.5	57
110	Phase Diagram and High-Temperature Superconductivity of Compressed Selenium Hydrides. <i>Scientific Reports</i> , <b>2015</b> , 5, 15433	4.9	56
109	Bismuth and antimony-based oxyhalides and chalcogenides as potential optoelectronic materials. <i>Npj Computational Materials</i> , <b>2018</b> , 4,	10.9	55
108	Ab initio prediction of superconductivity in molecular metallic hydrogen under high pressure. <i>Solid State Communications</i> , <b>2007</b> , 141, 610-614	1.6	55
107	Bulk heterojunction gifts bismuth-based lead-free perovskite solar cells with record efficiency. <i>Nano Energy</i> , <b>2020</b> , 68, 104362	17.1	54
106	Electronic structure and thermoelectric properties of layered PbSe-WSe <sub>2</sub> materials. <i>Physical Review B</i> , <b>2009</b> , 80,	3.3	52

105	Computer-Assisted Inverse Design of Inorganic Electrides. <i>Physical Review X</i> , <b>2017</b> , 7,	9.1	51
104	Proton-transfer-induced 3D/2D hybrid perovskites suppress ion migration and reduce luminance overshoot. <i>Nature Communications</i> , <b>2020</b> , 11, 3378	17.4	51
103	Experimental Identification of Critical Condition for Drastically Enhancing Thermoelectric Power Factor of Two-Dimensional Layered Materials. <i>Nano Letters</i> , <b>2018</b> , 18, 7538-7545	11.5	50
102	Ultrastable Lead-Free Double Perovskite Photodetectors with Imaging Capability. <i>Advanced Materials Interfaces</i> , <b>2019</b> , 6, 1900188	4.6	47
101	Ultrahigh-Performance Optoelectronics Demonstrated in Ultrathin Perovskite-Based Vertical Semiconductor Heterostructures. <i>ACS Nano</i> , <b>2019</b> , 13, 7996-8003	16.7	45
100	Electronic structure and thermoelectric properties: PbBi <sub>2</sub> Te <sub>4</sub> and related intergrowth compounds. <i>Physical Review B</i> , <b>2010</b> , 81,	3.3	45
99	Genomic design of strong direct-gap optical transition in Si/Ge core/multishell nanowires. <i>Nano Letters</i> , <b>2012</b> , 12, 984-91	11.5	43
98	N <sub>2</sub> H: a novel polymeric hydronitrogen as a high energy density material. <i>Journal of Materials Chemistry A</i> , <b>2015</b> , 3, 4188-4194	13	42
97	Phonon instabilities in rocksalt AgCl and AgBr under pressure studied within density functional theory. <i>Physical Review B</i> , <b>2006</b> , 74,	3.3	42
96	Electronic structure of Ba(Fe,Ru) <sub>2</sub> As <sub>2</sub> and Sr(Fe,Ir) <sub>2</sub> As <sub>2</sub> alloys. <i>Physical Review B</i> , <b>2009</b> , 79,	3.3	41
95	Dielectric Behavior as a Screen in Rational Searches for Electronic Materials: Metal Pnictide Sulfosalts. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 18058-18065	16.4	40
94	First-principles study of the lattice dynamics, thermodynamic properties and electron-phonon coupling of YB <sub>6</sub> . <i>Physical Review B</i> , <b>2007</b> , 76,	3.3	39
93	Electronic structure, localization, and spin-state transition in Cu-substituted FeSe:Fe <sub>1-x</sub> Cu <sub>x</sub> Se. <i>Physical Review B</i> , <b>2010</b> , 81,	3.3	38
92	Phonon and elastic instabilities in rocksalt alkali hydrides under pressure: First-principles study. <i>Physical Review B</i> , <b>2007</b> , 75,	3.3	37
91	Density functional study of the overdoped iron chalcogenide TlFe <sub>2</sub> Se <sub>2</sub> with ThCr <sub>2</sub> Si <sub>2</sub> structure. <i>Physical Review B</i> , <b>2009</b> , 79,	3.3	35
90	Electronic structures, lattice dynamics, and electron-phonon coupling of simple cubic Ca under pressure. <i>Solid State Communications</i> , <b>2008</b> , 146, 181-185	1.6	35
89	CaCl <sub>2</sub> -type high-pressure phase of magnesium hydride predicted by ab initio phonon calculations. <i>Physical Review B</i> , <b>2007</b> , 75,	3.3	33
88	Genetic design of enhanced valley splitting towards a spin qubit in silicon. <i>Nature Communications</i> , <b>2013</b> , 4, 2396	17.4	32

- 87 Bottom-up growth of homogeneous Moiré superlattices in bismuth oxychloride spiral nanosheets. *Nature Communications*, **2019**, 10, 4472 17.4 31
- 86 Discovery and ramifications of incidental Magn $\pi$  phase generation and release from industrial coal-burning. *Nature Communications*, **2017**, 8, 194 17.4 30
- 85 Rod-shaped thiocyanate-induced abnormal band gap broadening in SCN $\pi$ -doped CsPbBr $\pi$  perovskite nanocrystals. *Nano Research*, **2018**, 11, 2715-2723 10 30
- 84 ATLAS: A real-space finite-difference implementation of orbital-free density functional theory. *Computer Physics Communications*, **2016**, 200, 87-95 4.2 29
- 83 Cd-Rich Alloyed CsPb Cd Br Perovskite Nanorods with Tunable Blue Emission and Fermi Levels Fabricated through Crystal Phase Engineering. *Advanced Science*, **2020**, 7, 2000930 13.6 28
- 82 Spontaneous low-temperature crystallization of  $\pi$ -APbI $\pi$  for highly efficient perovskite solar cells. *Science Bulletin*, **2019**, 64, 1608-1616 10.6 27
- 81 Artificial control of in-plane anisotropic photoelectricity in monolayer MoS $\pi$ . *Applied Materials Today*, **2019**, 15, 203-211 6.6 27
- 80 Tuning optical properties of transparent conducting barium stannate by dimensional reduction. *APL Materials*, **2015**, 3, 011102 5.7 27
- 79 Intrinsic Transparent Conductors without Doping. *Physical Review Letters*, **2015**, 115, 176602 7.4 26
- 78 Pressure-induced enhancement of electron-phonon coupling in superconducting CaC $\pi$  from first principles. *Physical Review B*, **2006**, 74, 3.3 25
- 77 Stacking Effects on Electron-Phonon Coupling in Layered Hybrid Perovskites Microstrain Manipulation. *ACS Nano*, **2020**, 14, 5806-5817 16.7 24
- 76 Interlayer coupling in two-dimensional semiconductor materials. *Semiconductor Science and Technology*, **2018**, 33, 093001 1.8 23
- 75 Design of ternary alkaline-earth metal Sn(II) oxides with potential good p-type conductivity. *Journal of Materials Chemistry C*, **2016**, 4, 4592-4599 7.1 23
- 74 Anatase (101)-like Structural Model Revealed for Metastable Rutile TiO(011) Surface. *ACS Applied Materials & Interfaces*, **2017**, 9, 7891-7896 9.5 22
- 73 Density functional study of the electronic structure and magnetism of LaFeAsO alloyed with Zn. *Physical Review B*, **2009**, 80, 3.3 22
- 72 Dimension Engineering of High-Quality InAs Nanostructures on a Wafer Scale. *Nano Letters*, **2019**, 19, 1632-1642 11.5 22
- 71 Imaging of the Atomic Structure of All-Inorganic Halide Perovskites. *Journal of Physical Chemistry Letters*, **2020**, 11, 818-823 6.4 21
- 70 High-pressure phase transformations in CaH $\pi$ . *Journal of Physics Condensed Matter*, **2008**, 20, 045211 1.8 20

69	First-principles study of the pressure-induced rutile to CaCl <sub>2</sub> phase transition in MgF <sub>2</sub> . <i>Solid State Communications</i> , <b>2008</b> , 145, 283-287	1.6	20
68	Halide Homogenization for High-Performance Blue Perovskite Electroluminescence. <i>Research</i> , <b>2020</b> , 2020, 9017871	7.8	20
67	New Polymorphs of 2D Indium Selenide with Enhanced Electronic Properties. <i>Advanced Functional Materials</i> , <b>2020</b> , 30, 2001920	15.6	19
66	Computational functionality-driven design of semiconductors for optoelectronic applications. <i>Information Materials</i> , <b>2020</b> , 2, 879-904	23.1	19
65	High-throughput computational materials screening and discovery of optoelectronic semiconductors. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , <b>2021</b> , 11,	7.9	19
64	Design of Mixed-Cation Tri-Layered Pb-Free Halide Perovskites for Optoelectronic Applications. <i>Advanced Electronic Materials</i> , <b>2019</b> , 5, 1900234	6.4	18
63	Intrinsic ultralow lattice thermal conductivity of the unfilled skutterudite FeSb <sub>3</sub> . <i>Physical Review B</i> , <b>2016</b> , 94,	3.3	18
62	Color Tunable Self-Trapped Emissions from Lead-Free All Inorganic IA-IB Bimetallic Halides Cs-Ag-X (X = Cl, Br, I). <i>Small</i> , <b>2020</b> , 16, e2004272	11	18
61	Construction of crystal structure prototype database: methods and applications. <i>Journal of Physics Condensed Matter</i> , <b>2017</b> , 29, 165901	1.8	17
60	Possible superconductivity in Fe-Sb based materials: Density functional study of LiFeSb. <i>Physical Review B</i> , <b>2008</b> , 78,	3.3	17
59	Sn(II)-Containing Phosphates as Optoelectronic Materials. <i>Chemistry of Materials</i> , <b>2017</b> , 29, 2459-2465	9.6	16
58	Absence of intrinsic spin splitting in one-dimensional quantum wires of tetrahedral semiconductors. <i>Physical Review B</i> , <b>2011</b> , 84,	3.3	15
57	Impact of organic molecule rotation on the optoelectronic properties of hybrid halide perovskites. <i>Physical Review Materials</i> , <b>2019</b> , 3,	3.2	15
56	Extraordinary Temperature Dependent Second Harmonic Generation in Atomically Thin Layers of Transition-Metal Dichalcogenides. <i>Advanced Optical Materials</i> , <b>2020</b> , 8, 2000441	8.1	15
55	Effects of manganese doping on the structure evolution of small-sized boron clusters. <i>Journal of Physics Condensed Matter</i> , <b>2017</b> , 29, 265401	1.8	14
54	Observation of excitonic series in monolayer and few-layer black phosphorus. <i>Physical Review B</i> , <b>2020</b> , 101,	3.3	14
53	From Distortion to Disconnection: Linear Alkyl Diammonium Cations Tune Structure and Photoluminescence of Lead Bromide Perovskites. <i>Advanced Optical Materials</i> , <b>2020</b> , 8, 1902051	8.1	14
52	The birth of a type-II nanostructure: carrier localization and optical properties of isoelectronically doped CdSe:Te nanocrystals. <i>ACS Nano</i> , <b>2012</b> , 6, 8325-34	16.7	14



51	Switchable Out-of-Plane Polarization in 2D LiAlTe <sub>2</sub> . <i>Advanced Electronic Materials</i> , <b>2019</b> , 5, 1900089	6.4	13
50	Stable zero-dimensional cesium indium bromide hollow nanocrystals emitting blue light from self-trapped excitons. <i>Nano Today</i> , <b>2021</b> , 38, 101153	17.9	13
49	Band structure engineering through van der Waals heterostructuring superlattices of two-dimensional transition metal dichalcogenides. <i>Information Materials</i> , <b>2021</b> , 3, 201-211	23.1	13
48	Halogen Substitution in Zero-Dimensional Mixed Metal Halides toward Photoluminescence Modulation and Enhanced Quantum Yield. <i>Advanced Optical Materials</i> , <b>2020</b> , 8, 2000418	8.1	13
47	First-principle high-throughput calculations of carrier effective masses of two-dimensional transition metal dichalcogenides. <i>Journal of Semiconductors</i> , <b>2018</b> , 39, 072001	2.3	12
46	First-principles investigation of structural and electronic properties of oxygen adsorbing phosphorene. <i>Progress in Natural Science: Materials International</i> , <b>2019</b> , 29, 316-321	3.6	11
45	Rational design of new phases of tin monosulfide by first-principles structure searches. <i>Science China: Physics, Mechanics and Astronomy</i> , <b>2018</b> , 61, 1	3.6	11
44	Enhanced Optical Emission from 2D InSe Bent onto Si-Pillars. <i>Advanced Optical Materials</i> , <b>2020</b> , 8, 2000888	8.8	10
43	Excitons and excitonic fine structures in Si nanowires: Prediction of an electronic state crossover with diameter changes. <i>Physical Review B</i> , <b>2011</b> , 84,	3.3	10
42	Van der Waals SnSe <sub>2</sub> (1-x)S <sub>2x</sub> Alloys: Composition-Dependent Bowing Coefficient and Electron-Phonon Interaction. <i>Advanced Functional Materials</i> , <b>2020</b> , 30, 1908092	15.6	10
41	Stability, electronic structures and thermoelectric properties of binary ZnSb materials. <i>Journal of Materials Chemistry C</i> , <b>2016</b> , 4, 11305-11312	7.1	10
40	Molecular engineering towards efficient white-light-emitting perovskite. <i>Nature Communications</i> , <b>2021</b> , 12, 4890	17.4	10
39	Metal Halide Semiconductors beyond Lead-Based Perovskites for Promising Optoelectronic Applications. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 10532-10550	6.4	9
38	Alternative Lone-Pair ns <sup>2</sup> -Cation-Based Semiconductors beyond Lead Halide Perovskites for Optoelectronic Applications. <i>Advanced Materials</i> , <b>2021</b> , 33, e2008574	24	9
37	Stable Cesium-Rich Formamidinium/Cesium Pure-Iodide Perovskites for Efficient Photovoltaics. <i>ACS Energy Letters</i> , <b>2021</b> , 6, 2735-2741	20.1	9
36	Sn <sub>2</sub> Se <sub>3</sub> : A conducting crystalline mixed valent phase change memory compound. <i>Journal of Applied Physics</i> , <b>2017</b> , 121, 225106	2.5	8
35	Reinterpretation of the expected electronic density of states of semiconductor nanowires. <i>Nano Letters</i> , <b>2015</b> , 15, 88-95	11.5	8
34	New stable ternary alkaline-earth metal Pb(II) oxides: Ca/Sr/BaPb <sub>2</sub> O <sub>3</sub> and BaPbO <sub>2</sub> . <i>Physical Review Materials</i> , <b>2017</b> , 1,	3.2	8



33	JAMIP: an artificial-intelligence aided data-driven infrastructure for computational materials informatics. <i>Science Bulletin</i> , <b>2021</b> , 66, 1973-1985	10.6	8
32	Computational Design of Mixed-Valence Tin Sulfides as Solar Absorbers. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2019</b> , 11, 24867-24875	9.5	7
31	Collective-Goldstone-mode-induced ultralow lattice thermal conductivity in Sn-filled skutterudite SnFe <sub>4</sub> Sb <sub>12</sub> . <i>Physical Review B</i> , <b>2018</b> , 97,	3.3	6
30	Pb <sub>5</sub> Sb <sub>8</sub> S <sub>17</sub> quantum dot-sensitized solar cells with an efficiency of 6% under 0.05 sun: Theoretical and experimental studies. <i>Progress in Photovoltaics: Research and Applications</i> , <b>2018</b> , 26, 205-213	6.8	6
29	Rashba band splitting in two-dimensional Ruddlesden-Popper halide perovskites. <i>Journal of Applied Physics</i> , <b>2020</b> , 128, 175101	2.5	5
28	Perovskite Photovoltaics: Pseudohalide-Induced Recrystallization Engineering for CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> Film and Its Application in Highly Efficient Inverted Planar Heterojunction Perovskite Solar Cells (Adv. Funct. Mater. 2/2018). <i>Advanced Functional Materials</i> , <b>2018</b> , 28, 1870013	15.6	5
27	Dopability of divalent tin containing phosphates for p-type transparent conductors. <i>Physical Review Materials</i> , <b>2019</b> , 3,	3.2	5
26	Pressure-Tailored Band Engineering for Significant Enhancements in the Photoelectric Performance of CsI <sub>3</sub> in the Optical Communication Waveband. <i>Advanced Functional Materials</i> , <b>2018</b> , 28, 180636	15.6	5
25	Structural, Thermodynamical and Electronic Properties of All-Inorganic Lead Halide Perovskites. <i>Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica</i> , <b>2020</b> , 2007015-0	3.8	5
24	Diverse electronic properties of 2D layered Se-containing materials composed of quasi-1D atomic chains. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 2122-2129	3.6	4
23	The Introduction of Defects in Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> and Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> -Assisted Reduction of Graphene Oxide for Highly Selective Detection of ppb-Level NO <sub>2</sub> . <i>Advanced Functional Materials</i> , <b>2018</b> , 28, 180959	15.6	4
22	Discovery of New Polymorphs of Gallium Oxides with Particle Swarm Optimization-Based Structure Searches. <i>Advanced Electronic Materials</i> , <b>2020</b> , 6, 2000119	6.4	3
21	Phase transition pathway of hybrid halide perovskites under compression: Insights from first-principles calculations. <i>Physical Review Materials</i> , <b>2021</b> , 5,	3.2	3
20	High-throughput computational material screening of the cycloalkane-based two-dimensional DionJacobson halide perovskites for optoelectronics. <i>Chinese Physics B</i> , <b>2022</b> , 31, 037104	1.2	3
19	Electronic structure of CsFe <sub>2</sub> Sb <sub>2</sub> and its alloy with cobalt: A magnetic compound related to the iron superconductors. <i>Physical Review B</i> , <b>2010</b> , 81,	3.3	2
18	Optical emission enhancement of bent InSe thin films. <i>Science China Information Sciences</i> , <b>2021</b> , 64, 1	3.4	2
17	Electronic and optical properties of tapered tetrahedral semiconductor nanocrystals. <i>Nanotechnology</i> , <b>2021</b> , 32,	3.4	2
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15	White Light-Emitting Diodes: High Color-Rendering Index and Stable White Light-Emitting Diodes by Assembling Two Broadband Emissive Self-Trapped Excitons (Adv. Mater. 2/2021). <i>Advanced Materials</i> , <b>2021</b> , 33, 2170010	24	2
14	Evaluation of performance of machine learning methods in mining structure-property data of halide perovskite materials. <i>Chinese Physics B</i> ,	1.2	2
13	Global instability index as a crystallographic stability descriptor of halide and chalcogenide perovskites. <i>Journal of Energy Chemistry</i> , <b>2022</b> , 70, 1-8	12	2
12	Proton Transfer-Driven Modification of 3D Hybrid Perovskites to Form Oriented 2D Ruddlesden-Popper Phases. <i>Small Science</i> , <b>2022</b> , 2, 2100114		2
11	Rational Design of Additive with Suitable Functional Groups Toward High-Quality FA 0.75 MA 0.25 SnI 3 Films and Solar Cells. <i>Solar Rrl</i> ,2100800	7.1	1
10	Stability and electronic properties of two-dimensional metal-organic perovskites in Janus phase. <i>APL Materials</i> , <b>2021</b> , 9, 111105	5.7	1
9	Radiative parameters of high-lying levels in neutral rhodium. <i>Monthly Notices of the Royal Astronomical Society</i> , <b>2021</b> , 503, 5085-5090	4.3	1
8	Computational Design of Optoelectronic Semiconductor Materials <b>2018</b> ,		1
7	Temperature-induced phase transition of two-dimensional semiconductor GaTe. <i>Chinese Physics B</i> , <b>2021</b> , 30, 016402	1.2	1
6	Controlled Synthesis of Pure-Phase GaAs Nanowires through Shear Tension. <i>ACS Photonics</i> , <b>2021</b> , 8, 2886-2897	6.3	0
5	Discovery of New Phases of Bismuth Oxyselenide Semiconductor Bi2OSe2 by Global Structure Search Approach. <i>Advanced Theory and Simulations</i> , <b>2021</b> , 4, 2000316	3.5	0
4	The Introduction of Defects in Ti 3 C 2 T x and Ti 3 C 2 T x -Assisted Reduction of Graphene Oxide for Highly Selective Detection of ppb-Level NO 2 (Adv. Funct. Mater. 15/2022). <i>Advanced Functional Materials</i> , <b>2022</b> , 32, 2270091	15.6	0
3	Entropy-Driven Stabilization of Multielement Halide Double-Perovskite Alloys. <i>Journal of Physical Chemistry Letters</i> ,5017-5024	6.4	0
2	Electronic Structure, Magnetism and Spin-Fluctuations in Fe-As Based Superconductors. <i>Materials Research Society Symposia Proceedings</i> , <b>2008</b> , 1148, 1		
1	Radiative lifetimes, branching fractions, and oscillator strengths for highly excited levels in singly ionized tantalum (Ta ii). <i>Monthly Notices of the Royal Astronomical Society</i> , <b>2022</b> , 510, 4808-4818	4.3	