

Mao-Hua Du

List of Publications by Year in descending order

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169
papers

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28274

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times ranked

11702
citing authors

#	ARTICLE	IF	CITATIONS
1	Density Functional Study of LaFeAsO : A Low Carrier Density Superconductor Near Itinerant Magnetism. <i>Physical Review Letters</i> , 2008, 100, 237003.	7.8	1,049
2	Giant anharmonic phonon scattering in PbTe. <i>Nature Materials</i> , 2011, 10, 614-619.	27.5	561
3	Efficient carrier transport in halide perovskites: theoretical perspectives. <i>Journal of Materials Chemistry A</i> , 2014, 2, 9091-9098.	10.3	414
4	First-principles study of native defects in anatase TiO_2 . <i>Physical Review B</i> , 2006, 73, .	3.2	346
5	Density Functional Calculations of Native Defects in $\text{CH}_3\text{NH}_3\text{PbI}_3$: Effects of Spin-Orbit Coupling and Self-Interaction Error. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 1461-1466.	4.6	301
6	Low dimensional metal halide perovskites and hybrids. <i>Materials Science and Engineering Reports</i> , 2019, 137, 38-65.	31.8	300
7	Coherent Electron Transport through an Azobenzene Molecule: A Light-Driven Molecular Switch. <i>Physical Review Letters</i> , 2004, 92, 158301.	7.8	249
8	Bulk Separative Enrichment in Metallic or Semiconducting Single-Walled Carbon Nanotubes. <i>Nano Letters</i> , 2003, 3, 1245-1249.	9.1	246
9	A Zero-Dimensional Organic Seesaw-Shaped Tin Bromide with Highly Efficient Strongly Stokes-Shifted Deep-Red Emission. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 1021-1024.	13.8	219
10	Chemical trends of Mn^{4+} emission in solids. <i>Journal of Materials Chemistry C</i> , 2014, 2, 2475-2481.	5.5	214
11	Facile Preparation of Light Emitting Organic Metal Halide Crystals with Near-Unity Quantum Efficiency. <i>Chemistry of Materials</i> , 2018, 30, 2374-2378.	6.7	193
12	Near-Unity Photoluminescence Quantum Yield in Blue-Emitting $\text{Cs}_3\text{Cu}_2\text{Br}_5$ (0% Bi^{3+}). <i>ACS Applied Electronic Materials</i> , 2019, 1, 269-274.	4.3	184
13	Topological Insulator Behavior of Bi_2Te_3 . <i>Physical Review Applied</i> , 2015, 3, .	3.8	178
14	Unraveling luminescence mechanisms in zero-dimensional halide perovskites. <i>Journal of Materials Chemistry C</i> , 2018, 6, 6398-6405.	5.5	168
15	Large dielectric constant, high acceptor density, and deep electron traps in perovskite solar cell material CsGeI_3 . <i>Journal of Materials Chemistry A</i> , 2016, 4, 13852-13858.	10.3	148
16	Bright Luminescence from Nontoxic CsCu_2X_3 (X = Cl, Br, I). , 2019, 1, 459-465.		148
17	Hybrid Organic-Inorganic Halides ($\text{C}_5\text{H}_7\text{N}_2$) $_2\text{MBr}_4$ (M = Hg, Zn) with High Color Rendering Index and High-Efficiency White-Light Emission. <i>Chemistry of Materials</i> , 2019, 31, 2983-2991.	6.7	143
18	Fast Diffusion of Native Defects and Impurities in Perovskite Solar Cell Material $\text{CH}_3\text{NH}_3\text{PbI}_3$. <i>Chemistry of Materials</i> , 2016, 28, 4349-4357.	6.7	139

#	ARTICLE	IF	CITATIONS
19	Formation and Diffusion of Metal Impurities in Perovskite Solar Cell Material $\text{CH}_3\text{NH}_3\text{PbI}_3$: Implications on Solar Cell Degradation and Choice of Electrode. <i>Advanced Science</i> , 2018, 5, 1700662.	11.2	130
20	A One-Dimensional Organic Lead Chloride Hybrid with Excitation-Dependent Broadband Emissions. <i>ACS Energy Letters</i> , 2018, 3, 1443-1449.	17.4	124
21	Shallow halogen vacancies in halide optoelectronic materials. <i>Physical Review B</i> , 2014, 90, .	3.2	119
22	Green Emitting Single-Crystalline Bulk Assembly of Metal Halide Clusters with Near-Unity Photoluminescence Quantum Efficiency. <i>ACS Energy Letters</i> , 2019, 4, 1579-1583.	17.4	117
23	Electronic structure and magnetism in BaMn_2 <i>Physical Review B</i> , 2009, 79, .	3.2	112
24	First principles study of the graphene/Ru(0001) interface. <i>Journal of Chemical Physics</i> , 2009, 130, 074705.	3.0	111
25	Emission Trend of Multiple Self-Trapped Excitons in Luminescent 1D Copper Halides. <i>ACS Energy Letters</i> , 2020, 5, 464-469.	17.4	111
26	Intrinsic Defect Properties in Halide Double Perovskites for Optoelectronic Applications. <i>Physical Review Applied</i> , 2018, 10, .	3.8	109
27	Reaching 90% Photoluminescence Quantum Yield in One-Dimensional Metal Halide $\text{C}_4\text{N}_2\text{H}_{14}\text{PbBr}_4$ by Pressure-Suppressed Nonradiative Loss. <i>Journal of the American Chemical Society</i> , 2020, 142, 16001-16006.	13.7	109
28	K_2CuX_3 (X = Cl, Br): All-Inorganic Lead-Free Blue Emitters with Near-Unity Photoluminescence Quantum Yield. <i>Chemistry of Materials</i> , 2020, 32, 6197-6205.	6.7	109
29	Influence of defects and dopants on the photovoltaic performance of Bi_2S_3 : first-principles insights. <i>Journal of Materials Chemistry A</i> , 2017, 5, 6200-6210.	10.3	97
30	Deciphering Halogen Competition in Organometallic Halide Perovskite Growth. <i>Journal of the American Chemical Society</i> , 2016, 138, 5028-5035.	13.7	92
31	Bulk Assembly of Zero-Dimensional Organic Lead Bromide Hybrid with Efficient Blue Emission. , 2019, 1, 594-598.		92
32	First-Principles Prediction of Thermodynamically Stable Two-Dimensional Electrides. <i>Journal of the American Chemical Society</i> , 2016, 138, 15336-15344.	13.7	91
33	Structural and crystal chemical properties of rare-earth titanate pyrochlores. <i>Journal of Alloys and Compounds</i> , 2014, 605, 63-70.	5.5	90
34	Rb_2CuX_3 (X = Cl, Br): 1D All-Inorganic Copper Halides with Ultrabright Blue Emission and Up-Conversion Photoluminescence. <i>Advanced Optical Materials</i> , 2020, 8, 1901338.	7.3	86
35	Anionic and Hidden Hydrogen in ZnO. <i>Physical Review Letters</i> , 2011, 106, 115502.	7.8	84
36	Bismuth chalcogenides and oxyhalides as optoelectronic materials. <i>Physical Review B</i> , 2016, 93, .	3.2	82

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37	Water-silica surface interactions: A combined quantum-classical molecular dynamic study of energetics and reaction pathways. <i>Journal of Chemical Physics</i> , 2003, 119, 6418-6422.	3.0	78
38	Energy transport and scintillation of cerium-doped elpasolite Cs_2LiYCl_6 : Hybrid density functional calculations. <i>Physical Review B</i> , 2012, 86, .	3.2	78
39	Synthesis, Crystal and Electronic Structures, and Optical Properties of $(CH_3)_3NH_2 \cdot CdX_4$ (X = Cl, Br, I). <i>Inorganic Chemistry</i> , 2017, 56, 13878-13888.	4.0	78
40	Bulk assembly of organic metal halide nanotubes. <i>Chemical Science</i> , 2017, 8, 8400-8404.	7.4	76
41	Enhanced Born charge and proximity to ferroelectricity in thallium halides. <i>Physical Review B</i> , 2010, 81, .	3.2	72
42	OD and 2D: The Cases of Phenylethylammonium Tin Bromide Hybrids. <i>Chemistry of Materials</i> , 2020, 32, 4692-4698.	6.7	72
43	Impurity-bound small polarons in ZnO: Hybrid density functional calculations. <i>Physical Review B</i> , 2009, 80, .	3.2	71
44	Broadband Emission in Hybrid Organic-Inorganic Halides of Group 12 Metals. <i>ACS Omega</i> , 2018, 3, 18791-18802.	3.5	70
45	Trapped-Dopant Model of Doping in Semiconductor Nanocrystals. <i>Nano Letters</i> , 2008, 8, 2878-2882.	9.1	69
46	Tuning Fermi Levels in Intrinsic Antiferromagnetic Topological Insulators $MnBi_2Te_4$ and $MnBi_4Te_7$ by Defect Engineering and Chemical Doping. <i>Advanced Functional Materials</i> , 2021, 31, 2006516.	14.9	68
47	Chemical instability leads to unusual chemical-potential-independent defect formation and diffusion in perovskite solar cell material $CH_3NH_3PbI_3$. <i>Journal of Materials Chemistry A</i> , 2016, 4, 16975-16981.	10.3	67
48	Zintl-phase compounds with $SnSb_4$ anions: Electronic structure and thermoelectric properties. <i>Physical Review B</i> , 2010, 81, .	4.2	66
49	Zero-dimensional Cs_4EuX_6 (X = Br, I) all-inorganic perovskite single crystals for gamma-ray spectroscopy. <i>Journal of Materials Chemistry C</i> , 2018, 6, 6647-6655.	5.5	66
50	Bulk Assembly of Corrugated 1D Metal Halides with Broadband Yellow Emission. <i>Advanced Optical Materials</i> , 2019, 7, 1801474.	7.3	65
51	Spin Ice: Magnetic Excitations without Monopole Signatures Using Muon Spin Rotation. <i>Physical Review Letters</i> , 2011, 107, 207207.	7.8	60
52	Real-time Observation of Order-Disorder Transformation of Organic Cations Induced Phase Transition and Anomalous Photoluminescence in Hybrid Perovskites. <i>Advanced Materials</i> , 2018, 30, e1705801.	21.0	60
53	Impact of metal lone pair on luminescence quantum efficiency in low-dimensional halide perovskites. <i>Physical Review Materials</i> , 2019, 3, .	2.4	60
54	Carrier compensation in semi-insulating CdTe: First-principles calculations. <i>Physical Review B</i> , 2008, 77, .	3.2	59

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55	A Zero-Dimensional Organic Seesaw-Shaped Tin Bromide with Highly Efficient Strongly Stokes-Shifted Deep-Red Emission. <i>Angewandte Chemie</i> , 2018, 130, 1033-1036.	2.0	58
56	What causes high resistivity in CdTe. <i>New Journal of Physics</i> , 2012, 14, 063020.	2.9	57
57	Highly Efficient Broad-Band Luminescence Involving Organic and Inorganic Molecules in a Zero-Dimensional Hybrid Lead Chloride. <i>Journal of Physical Chemistry C</i> , 2019, 123, 22470-22477.	3.1	57
58	First-Principles Prediction of Icosahedral Quantum Dots for Tetravalent Semiconductors. <i>Physical Review Letters</i> , 2004, 93, .	7.8	55
59	Observation of Nanoscale Morphological and Structural Degradation in Perovskite Solar Cells by in Situ TEM. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 32333-32340.	8.0	54
60	Hydrolysis of a two-membered silica ring on the amorphous silica surface. <i>Journal of Chemical Physics</i> , 2004, 120, 1044-1054.	3.0	53
61	Flat bands in the CoSn-type compounds. <i>Physical Review B</i> , 2020, 102, .	3.2	52
62	Tuning magnetic order in the van der Waals metal $\text{Fe}_{2-x}\text{Co}_x\text{Te}$ by cobalt substitution. <i>Physical Review Materials</i> , 2020, 4, .	2.4	52
63	Discrete Electronic Bands in Semiconductors and Insulators: Potential High-Light-Yield Scintillators. <i>Physical Review Applied</i> , 2015, 3, .	3.8	51
64	Photo-Oxidation of Polyhydroxyl Molecules on TiO ₂ Surfaces: From Hole Scavenging to Light-Induced Self-Assembly of TiO ₂ -Cyclodextrin Wires. <i>Physical Review Letters</i> , 2007, 98, 066102.	7.8	50
65	Native defects and oxygen and hydrogen-related defect complexes in CdTe: Density functional calculations. <i>Journal of Applied Physics</i> , 2008, 104, 093521.	2.5	50
66	Composition-Dependent Photoluminescence Properties and Anti-Counterfeiting Applications of A_2AgX_3 ($\text{A} = \text{Rb, Cs}$; $\text{X} = \text{Cl, Br, I}$). <i>Advanced Functional Materials</i> , 2021, 31, 2104941.	14.9	50
67	Crystal Synthesis and Frustrated Magnetism in Triangular Lattice CsRE_2Se_2 ($\text{RE} = \text{Lu}$): Quantum Spin Liquid Candidates CsCeSe_2 and CsYbSe_2 . <i>Physical Review Letters</i> , 2020, 2, 71-75.		49
68	Zero-Dimensional Hybrid Organic-Inorganic Indium Bromide with Blue Emission. <i>Inorganic Chemistry</i> , 2021, 60, 1045-1054.	4.0	48
69	Potential thermoelectric performance of hole-doped Cu_2O . <i>New Journal of Physics</i> , 2013, 15, 043029.	2.9	47
70	Deciphering the effect of traps on electronic charge transport properties of methylammonium lead tribromide perovskite. <i>Science Advances</i> , 2020, 6, .	10.3	47
71	Predicting the thermodynamic stability of double-perovskite halides from density functional theory. <i>APL Materials</i> , 2018, 6, .	5.1	42
72	Antisite Pairs Suppress the Thermal Conductivity of BAs. <i>Physical Review Letters</i> , 2018, 121, 105901.	7.8	41

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73	Electron-phonon superconductivity in LaNiPO. Physical Review B, 2008, 78, .	3.2	40
74	Enhanced Born charges in III-VI, $\frac{IV-VII}{2}$ and $\frac{V-VII}{3}$ Physical Review B, 2010, 82, .	3.2	40
75	Native defects in antiferromagnetic topological insulator $MnBi_2Te_4$ Physical Review Materials, 2020, 4, .	2.2	10
76	Stabilization mechanisms of polar surfaces: ZnO surfaces. Physical Review B, 2008, 78, .	3.2	37
77	Prospective high thermoelectric performance of the heavily p -doped half-Heusler compound CoVSn. Physical Review B, 2017, 95, .	3.2	37
78	First-principles study of native defects in TlBr: Carrier trapping, compensation, and polarization phenomenon. Journal of Applied Physics, 2010, 108, .	2.5	36
79	Bistability-Mediated Carrier Recombination at Light-Induced Boron-Oxygen Complexes in Silicon. Physical Review Letters, 2006, 97, 256602.	7.8	35
80	Mn ⁴⁺ emission in pyrochlore oxides. Journal of Luminescence, 2015, 157, 69-73.	3.1	35
81	Rb ₄ Ag ₂ BiBr ₉ : A Lead-Free Visible Light Absorbing Halide Semiconductor with Improved Stability. Inorganic Chemistry, 2019, 58, 4446-4455.	4.0	35
82	Crystal growth and scintillation properties of pure and Tl-doped Cs ₃ Cu ₂ I ₅ . Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2021, 991, 164963.	1.6	35
83	Properties of alkaline-earth-filled skutterudite antimonides: $Ca_2Fe_4Sb_{12}$		

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91	Manipulation of fullerene-induced impurity states in carbon peapods. Physical Review B, 2003, 68, .	3.2	25
92	DXcenters in GaAs and GaSb. Physical Review B, 2005, 72, .	3.2	25
93	Transport and optical properties of heavily hole-doped semiconductors BaCu ₂ Se ₂ and BaCu ₂ Te ₂ . Journal of Solid State Chemistry, 2011, 184, 2744-2750.	2.9	25
94	Design of High-Performance Lead-Free Quaternary Antiperovskites for Photovoltaics via Ion Type Inversion and Anion Ordering. Journal of the American Chemical Society, 2021, 143, 12369-12379.	13.7	24
95	Determination of miscibility in MgO-ZnO nanocrystal alloys by x-ray absorption spectroscopy. Applied Physics Letters, 2011, 99, 261901.	3.3	23
96	Microscopic origin of multiple exciton emission in low-dimensional lead halide perovskites. Journal of Chemical Physics, 2019, 151, 181101.	3.0	23
97	Electronic structure engineering of elpasolites: Case of Cs ₂ AgYCl ₆ . Journal of Luminescence, 2013, 143, 710-714.	3.1	22
98	Scintillation Properties and Electronic Structures of the Intrinsic and Extrinsic Mixed Elpasolites $\text{Cs}_2\text{Mn}_2\text{Mn}_2\text{Mn}_2$	3.3	22
99	Scintillation Properties and Electronic Structures of the Intrinsic and Extrinsic Mixed Elpasolites Sb_3	3.2	21
100	Intense deep-red zero phonon line emission of Mn ⁴⁺ in double perovskite La ₄ Ti ₃ O ₁₂ . Physical Chemistry Chemical Physics, 2019, 21, 25108-25117.	2.8	21
101	AX centers in II-VI semiconductors: Hybrid functional calculations. Applied Physics Letters, 2011, 98, .	3.3	18
102	First principles study of native defects in InI. Journal of Applied Physics, 2011, 109, 113518.	2.5	17
103	Transparent interface between classical molecular dynamics and first-principles molecular dynamics. International Journal of Quantum Chemistry, 2003, 93, 1-8.	2.0	16
104	Chemical Trend of Transition-Metal Doping in WSe ₂ . Physical Review Applied, 2019, 12, .	3.8	16
105	Hydrogen in anion vacancies of semiconductors. Physical Review B, 2009, 79, .	3.2	15
106	Direct Evidence of Exciton-Exciton Annihilation in Single-Crystalline Organic Metal Halide Nanotube Assemblies. Journal of Physical Chemistry Letters, 2018, 9, 2164-2169.	4.6	15
107	(CH ₃ NH ₃) ₄ X ₄ ·H ₂ O (X=Cl, Br) and (CH ₃ NH ₃) ₄ AuCl ₄ : Low-Band Gap Lead-Free Layered Gold Halide Perovskite Materials. Chemistry - A European Journal, 2019, 25, 9875-9884.	3.3	15
108	Excitation Energies of Localized Correlated Defects via Quantum Monte Carlo: A Case Study of Mn ⁴⁺ -Doped Phosphors. Journal of Physical Chemistry Letters, 2019, 10, 67-74.	4.6	15

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109	Robust Ferromagnetism in Highly Strained SrCoO_3 . Physical Review X, 2020, 10, .	8.9	15
110	Adsorption-controlled growth of MnTe by molecular beam epitaxy exhibiting stoichiometry-controlled magnetism. Physical Review Materials, 2020, 4, .	2.4	15
111	Electronic structure, magnetism and superconductivity of layered iron compounds. Physica C: Superconductivity and Its Applications, 2009, 469, 886-889.	1.2	14
112	Crystal structure, electronic structure, temperature-dependent optical and scintillation properties of CsCe_2Br_7 . Journal of Materials Chemistry C, 2015, 3, 11366-11376.	5.5	14
113	$(\text{NH}_4)_2\text{AgX}_3$ (X = Br, I): 1D Silver Halides with Broadband White Light Emission and Improved Stability. ACS Materials Au, 2021, 1, 62-68.	6.0	14
114	Tuning the room temperature ferromagnetism in Fe_5GeTe_2 by arsenic substitution. 2D Materials, 2022, 9, 015013.	4.4	14
115	Hydrogen-Mediated Nitrogen Clustering in Dilute III-V Nitrides. Physical Review Letters, 2006, 97, 075503.	7.8	13
116	Bismuth-induced deep levels and carrier compensation in CdTe. Physical Review B, 2008, 78, .	3.2	13
117	First-principles study of back-contact effects on CdTe thin-film solar cells. Physical Review B, 2009, 80, .	3.2	13
118	Topological defects and the Staebler-Wronski effect in hydrogenated amorphous silicon. Applied Physics Letters, 2005, 87, 191903.	3.3	12
119	Crystal structure, electronic structure, optical and scintillation properties of self-activated Cs_4YbI_6 . Journal of Luminescence, 2018, 201, 460-465.	3.1	12
120	Quantum, classical, and multi-scale simulation of silica-water interaction: molecules, clusters, and extended systems. Journal of Computer-Aided Materials Design, 2006, 13, 161-183.	0.7	11
121	Defects in AlSb: A density functional study. Physical Review B, 2009, 79, .	3.2	11
122	Vibrational signatures of OTe and OTe-VCd in CdTe: A first-principles study. Computational Materials Science, 2010, 49, S242-S245.	3.0	11
123	Electronic structure, small polaron, and F center in LiCaAlF_6 . Journal of Applied Physics, 2012, 112, 123516.	2.5	11
124	Zero-dimensional metal oxide Li_4TiO_4 . Journal of Materials Chemistry C, 2019, 7, 5710-5715.	5.5	11
125	Additive-assisted synthesis and optoelectronic properties of $(\text{CH}_3\text{NH}_3)_4\text{BiI}_2$. Inorganic Chemistry Frontiers, 2020, 7, 1564-1572.	6.0	11
126	Crystal growth, density functional theory, and scintillation properties of $\text{Tl}_3\text{LnCl}_6:\text{Ce}^{3+}$ and $\text{TlLn}_2\text{Cl}_7:\text{Ce}^{3+}$ (Ln = Y, Gd). Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2021, 995, 165047.	1.6	11

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127	(C ₇ H ₁₁ N ₂) ₂ MBr ₄ (M=Cu, Zn): X-ray Sensitive OD Hybrid Metal Halides with Tunable Broadband Emission. European Journal of Inorganic Chemistry, 2022, 2022, e202100954.	2.0	11
128	DX centers in CdTe: A density functional study. Applied Physics Letters, 2008, 92, 181908.	3.3	10
129	Optoelectronic properties of candidate photovoltaic Cu ₂ PbSiS ₄ , Ag ₂ PbGeS ₄ and KAg ₂ SbS ₄ semiconductors. Journal of Alloys and Compounds, 2018, 746, 405-412.	5.5	10
130	Synthesis, crystal and electronic structures and optical properties of (HIm) ₂ Hg ₃ Cl ₈ and (HIm)HgI ₃ (HIm = imidazolium). Journal of Solid State Chemistry, 2018, 258, 551-558.	2.9	10
131	Doping Y ₂ O ₃ with Mn ⁴⁺ for energy-efficient lighting. Journal of Materials Chemistry C, 2018, 6, 4171-4176.	5.5	10
132	First principles study of O defects in CdSe. Physica B: Condensed Matter, 2012, 407, 2841-2845. Ternary chalcogenides	2.7	9
133	$C_{2}Z_{3}$	3.2	9
134	Impurity-induced deep centers in Tl ₆ Si ₄ . Journal of Applied Physics, 2017, 121, 145102. Thallium-based scintillators for high-resolution gamma-ray spectroscopy: Ce	2.5	9
135	$S_{3}Mo_{3}$ -doped Tl ₂ LaCl ₅ and Tl ₂ LaBr ₅	1.6	9
136	Intrinsic and complex defect engineering of quasi-one-dimensional ribbons $Sb_{2}S_{3}$ for photovoltaics performance. Physical Review Materials, 2021, 5, .	2.4	9
137	Effects of impurity doping on ionic conductivity and polarization phenomenon in TlBr. Applied Physics Letters, 2013, 102, 082102.	3.3	8
138	Electronic shell structures, self-trapped excitons, and defect-bound excitons in Li ₂ B ₁₂ H ₁₂ . Journal of Materials Chemistry C, 2019, 7, 14342-14349.	5.5	8
139	Role of Lithium Codoping in Enhancing the Scintillation Yield of Aluminate Garnets. Physical Review Applied, 2020, 13, .	3.8	8
140	Role of Polycyclic Aromatic Alkylammonium Cations in Tuning the Electronic Properties and Band Alignment of Two-Dimensional Hybrid Perovskite Semiconductors. Journal of Physical Chemistry Letters, 2021, 12, 9754-9760.	4.6	8
141	Li ₂ Se:Te as a neutron scintillator. Journal of Alloys and Compounds, 2015, 647, 906-910.	5.5	7
142	Native defects in Tl ₆ Si ₄ : Density functional calculations. Journal of Applied Physics, 2015, 117, .	2.5	7
143	TlSr ₂ 15:Eu ²⁺ A new high density scintillator for gamma-ray detection. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2021, 988, 164876.	1.6	7
144	Magnetic properties of the Shastry-Sutherland lattice material $BaNd_{2}$		

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145	Resistivity, carrier trapping, and polarization phenomenon in semiconductor radiation detection materials. Proceedings of SPIE, 2012, , .	0.8	6
146	High magnetocrystalline anisotropy in oxides with near cubic local environments. Applied Physics Letters, 2013, 102, .	3.3	6
147	First-principles study of impurities in TlBr. Journal of Applied Physics, 2012, 111, 073519.	2.5	5
148	Identification of oxygen defects in CdTe revisited: First-principles study. Journal of Applied Physics, 2014, 115, 203511.	2.5	5
149	(INVITED) First-principles calculations of quantum transitions at local centers. Optical Materials: X, 2020, 8, 100066.	0.8	5
150	Hierarchical excitations from correlated spin tetrahedra on the breathing pyrochlore lattice. Physical Review B, 2021, 103, .	3.2	5
151	Electronic structure, energy transport, and optical properties of halide scintillators. Proceedings of SPIE, 2012, , .	0.8	4
152	First principles calculations of Hydrogenâ€”Titanium vacancy complexes in SrTiO3. Ceramics International, 2013, 39, S273-S276.	4.8	4
153	Photophysical properties of zero-dimensional perovskites studied by PBE0 and GW+BSE methods. Journal of Applied Physics, 2021, 130, 203106.	2.5	4
154	First-principles study of defects and carrier compensation in semiconductor radiation detector materials. Materials Research Society Symposia Proceedings, 2009, 1164, 1.	0.1	3
155	Ba2TeO as an optoelectronic material: First-principles study. Journal of Applied Physics, 2015, 117, 195705.	2.5	3
156	Ion relaxation and hydrogen LVM in H-irradiated GaAsN. Physica B: Condensed Matter, 2006, 376-377, 583-586.	2.7	2
157	Chemical stability and Ce doping of LiMgAlF6 neutron scintillator. Journal of Alloys and Compounds, 2015, 622, 925-928.	5.5	2
158	Density functional studies of defects and defect-related luminescence in Mg3N2. Physical Review Materials, 2020, 4, .	2.4	2
159	Crystal growth, density functional theory, and scintillation properties of TMgX3 (X=Cl, Br, I). Chemical Physics, 2022, 558, 111535.	1.9	2
160	Surfaceâ€”Driven Evolution of the Anomalous Hall Effect in Magnetic Topological Insulator MnBi2Te4 Thin Films. Advanced Functional Materials, 2022, 32, .	14.9	2
161	Crossover in energy redistribution during C60@Xe144 surface impact. Physical Review B, 2001, 64, .	3.2	1
162	Unifying Chemical Bonding Models for Boranes. Materials Research Society Symposia Proceedings, 2007, 1038, 1.	0.1	1

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163	First-principles study of electronic structure, defects, and activators in LiCaAlF ₆ . , 2013, , .		1
164	Organohalide Perovskites: Real-Time Observation of Order-Disorder Transformation of Organic Cations Induced Phase Transition and Anomalous Photoluminescence in Hybrid Perovskites (Adv. Tj ETQq0 0 0 rg BT1/Overlook 10 Tf 50		0
165	Electronic Structure, Magnetism and Spin-Fluctuations in Fe-As Based Superconductors. Materials Research Society Symposia Proceedings, 2008, 1148, 1.	0.1	0
166	First-principles Study of Back Contact Effects on CdTe Thin Film Solar Cells. Materials Research Society Symposia Proceedings, 2010, 1268, 1.	0.1	0
167	Atomic-Scale Study of Intrinsic Defects Suppressing the Thermal Conductivity of Boron Arsenide. Microscopy and Microanalysis, 2019, 25, 942-943.	0.4	0
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