Mao-Hua Du

List of Publications by Year
in descending order

169	10,636	29994	34900
papers	citations	54 h-index	98 g-index

176	176	176	11702
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Density Functional Study of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>LaFeAsO</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^'</mml:mo><mml:mi>x</mi></mml:mrow></mml:msub></mml:math> mathvariant="normal">F</mml:mi><mml:mi>x</mml:mi></mml:msub></mml:math>: A Low Carrier Density Superconductor Near Itinerant Magnetism. Physical Review Letters, 2008, 100, 237003.	2.9	1,049
2	Giant anharmonic phonon scattering in PbTe. Nature Materials, 2011, 10, 614-619.	13.3	561
3	Efficient carrier transport in halide perovskites: theoretical perspectives. Journal of Materials Chemistry A, 2014, 2, 9091-9098.	5.2	414
4	First-principles study of native defects in anataseTiO2. Physical Review B, 2006, 73, .	1.1	346
5	Density Functional Calculations of Native Defects in CH₃NH₃PbI₃: Effects of Spinâ€“Orbit Coupling and Self-Interaction Error. Journal of Physical Chemistry Letters, 2015, 6, 1461-1466.	2.1	301
6	Low dimensional metal halide perovskites and hybrids. Materials Science and Engineering Reports, 2019, 137, 38-65.	14.8	300
7	Coherent Electron Transport through an Azobenzene Molecule: A Light-Driven Molecular Switch. Physical Review Letters, 2004, 92, 158301.	2.9	249
8	Bulk Separative Enrichment in Metallic or Semiconducting Single-Walled Carbon Nanotubes. Nano Letters, 2003, 3, 1245-1249.	4.5	246
9	A Zeroâ€Dimensional Organic Seesawâ€Shaped Tin Bromide with Highly Efficient Strongly Stokesâ€Shifted Deepâ€Red Emission. Angewandte Chemie - International Edition, 2018, 57, 1021-1024.	7.2	219
10	Chemical trends of Mn⁴⁺emission in solids. Journal of Materials Chemistry C, 2014, 2, 2475-2481.	2.7	214
11	Facile Preparation of Light Emitting Organic Metal Halide Crystals with Near-Unity Quantum Efficiency. Chemistry of Materials, 2018, 30, 2374-2378.	3.2	193
12	Near-Unity Photoluminescence Quantum Yield in Blue-Emitting Cs₃Cu₂Br_{5â€“x}I_x (0 â‰¤ x â‰¤ 5). ACS Applied Electronic Materials, 2019, 1, 269-274.	2.0	184
13	Engineering Thermoelectric Properties and Topological-Insulator Behavior: <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Bi</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Bi</mml:mi></mml:m. Physical Review Applied, 2015, 3, .	1.5	178
14	Unraveling luminescence mechanisms in zero-dimensional halide perovskites. Journal of Materials Chemistry C, 2018, 6, 6398-6405.	2.7	168
15	Large dielectric constant, high acceptor density, and deep electron traps in perovskite solar cell material CsGeI₃. Journal of Materials Chemistry A, 2016, 4, 13852-13858.	5.2	148
16	Bright Luminescence from Nontoxic CsCu₂X₃ (X = Cl, Br, I). , 2019, 1, 459-465.		148
17	Hybrid Organicâ€“Inorganic Halides (C₅H₇N₂)₂MBr₄ (M = Hg, Zn) with High Color Rendering Index and High-Efficiency White-Light Emission. Chemistry of Materials, 2019, 31, 2983-2991.	3.2	143
18	Fast Diffusion of Native Defects and Impurities in Perovskite Solar Cell Material CH₃NH₃PbI₃. Chemistry of Materials, 2016, 28, 4349-4357.	3.2	139

#	Article	IF	Citations
19	Formation and Diffusion of Metal Impurities in Perovskite Solar Cell Material CH₃NH₃PbI₃: Implications on Solar Cell Degradation and Choice of Electrode. Advanced Science, 2018, 5, 1700662.	5.6	130
20	A One-Dimensional Organic Lead Chloride Hybrid with Excitation-Dependent Broadband Emissions. ACS Energy Letters, 2018, 3, 1443-1449.	8.8	124
21	Shallow halogen vacancies in halide optoelectronic materials. Physical Review B, 2014, 90, .	1.1	119
22	Green Emitting Single-Crystalline Bulk Assembly of Metal Halide Clusters with Near-Unity Photoluminescence Quantum Efficiency. ACS Energy Letters, 2019, 4, 1579-1583.	8.8	117
23	Electronic structure and magnetism in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>BaMn</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>Physical Review B, 2009, 79, .	1.1	112
24	First principles study of the graphene/Ru(0001) interface. Journal of Chemical Physics, 2009, 130, 074705.	1.2	111
25	Emission Trend of Multiple Self-Trapped Excitons in Luminescent 1D Copper Halides. ACS Energy Letters, 2020, 5, 464-469.	8.8	111
26	Intrinsic Defect Properties in Halide Double Perovskites for Optoelectronic Applications. Physical Review Applied, 2018, 10, .	1.5	109
27	Reaching 90% Photoluminescence Quantum Yield in One-Dimensional Metal Halide C₄N₂H₁₄PbBr₄ by Pressure-Suppressed Nonradiative Loss. Journal of the American Chemical Society, 2020, 142, 16001-16006.	6.6	109
28	K₂CuX₃ (X = Cl, Br): All-Inorganic Lead-Free Blue Emitters with Near-Unity Photoluminescence Quantum Yield. Chemistry of Materials, 2020, 32, 6197-6205.	3.2	109
29	Influence of defects and dopants on the photovoltaic performance of Bi₂S₃: first-principles insights. Journal of Materials Chemistry A, 2017, 5, 6200-6210.	5.2	97
30	Deciphering Halogen Competition in Organometallic Halide Perovskite Growth. Journal of the American Chemical Society, 2016, 138, 5028-5035.	6.6	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. Journal of the American Chemical Society, 2016, 138, 15336-15344.	6.6	91
33	Structural and crystal chemical properties of rare-earth titanate pyrochlores. Journal of Alloys and Compounds, 2014, 605, 63-70.	2.8	90
34	Rb₂CuX₃ (X = Cl, Br): 1D Allâ€inorganic Copper Halides with Ultrabright Blue Emission and Upâ€Conversion Photoluminescence. Advanced Optical Materials, 2020, 8, 1901338.	3.6	86
35	Anionic and Hidden Hydrogen in ZnO. Physical Review Letters, 2011, 106, 115502.	2.9	84
36	Bismuth chalcohalides and oxyhalides as optoelectronic materials. Physical Review B, 2016, 93, .	1.1	82

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37	Waterâ€“silica surface interactions: A combined quantum-classical molecular dynamic study of energetics and reaction pathways. Journal of Chemical Physics, 2003, 119, 6418-6422.	1.2	78
38	Energy transport and scintillation of cerium-doped elpasolite Cs<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>LiYCl<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>6</mml:mn></mml:msub></mml:math>: Hybrid density functional calculations. Physical Review B, 2012, 86, .	1.1	78
39	Synthesis, Crystal and Electronic Structures, and Optical Properties of (CH₃NH₃)₂CdX₄ (X = Cl, Br, I). Inorganic Chemistry, 2017, 56, 13878-13888.	1.9	78
40	Bulk assembly of organic metal halide nanotubes. Chemical Science, 2017, 8, 8400-8404.	3.7	76
41	Enhanced Born charge and proximity to ferroelectricity in thallium halides. Physical Review B, 2010, 81, .	1.1	72
42	0D and 2D: The Cases of Phenylethylammonium Tin Bromide Hybrids. Chemistry of Materials, 2020, 32, 4692-4698.	3.2	72
43	Impurity-bound small polarons in ZnO: Hybrid density functional calculations. Physical Review B, 2009, 80, .	1.1	71
44	Broadband Emission in Hybrid Organicâ€“Inorganic Halides of Group 12 Metals. ACS Omega, 2018, 3, 18791-18802.	1.6	70
45	Trapped-Dopant Model of Doping in Semiconductor Nanocrystals. Nano Letters, 2008, 8, 2878-2882.	4.5	69
46	Tuning Fermi Levels in Intrinsic Antiferromagnetic Topological Insulators MnBi₂Te₄ and MnBi₄Te₇ by Defect Engineering and Chemical Doping. Advanced Functional Materials, 2021, 31, 2006516.	7.8	68
47	Chemical instability leads to unusual chemical-potential-independent defect formation and diffusion in perovskite solar cell material CH₃NH₃PbI₃. Journal of Materials Chemistry A, 2016, 4, 16975-16981.	5.2	67
48	Zintl-phase compounds with<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SnSb</mml:mtext></mml:mrow><mml:mn>4</mml:mn></mml:msub></mml:m anions: Electronic structure and thermoelectric properties. Physical Review B, 2010, 81, .	4.1	66
49	Zero-dimensional Cs₄EuX₆ (X = Br, I) all-inorganic perovskite single crystals for gamma-ray spectroscopy. Journal of Materials Chemistry C, 2018, 6, 6647-6655.	2.7	66
50	Bulk Assembly of Corrugated 1D Metal Halides with Broadband Yellow Emission. Advanced Optical Materials, 2019, 7, 1801474.	3.6	65
51	Spin Ice: Magnetic Excitations without Monopole Signatures Using Muon Spin Rotation. Physical Review Letters, 2011, 107, 207207.	2.9	60
52	Realâ€Time Observation of Orderâ€Disorder Transformation of Organic Cations Induced Phase Transition and Anomalous Photoluminescence in Hybrid Perovskites. Advanced Materials, 2018, 30, e1705801.	11.1	60
53	Impact of metal <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">n</mml:mi><mml:msup><mml:mrow><mml:mi mathvariant="normal">s</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msup></mml:mrow></mml:math> lone pair on luminescence quantum efficiency in low-dimensional halide perovskites. Physical Review Materials, 2019, 3, .	0.9	60
54	Carrier compensation in semi-insulating CdTe: First-principles calculations. Physical Review B, 2008, 77, .	1.1	59

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55	A Zeroâ€Dimensional Organic Seesawâ€Shaped Tin Bromide with Highly Efficient Strongly Stokesâ€Shifted Deepâ€Red Emission. Angewandte Chemie, 2018, 130, 1033-1036.	1.6	58
56	What causes high resistivity in CdTe. New Journal of Physics, 2012, 14, 063020.	1.2	57
57	Highly Efficient Broad-Band Luminescence Involving Organic and Inorganic Molecules in a Zero-Dimensional Hybrid Lead Chloride. Journal of Physical Chemistry C, 2019, 123, 22470-22477.	1.5	57
58	First-Principles Prediction of Icosahedral Quantum Dots for Tetravalent Semiconductors. Physical Review Letters, 2004, 93, .	2.9	55
59	Observation of Nanoscale Morphological and Structural Degradation in Perovskite Solar Cells by in Situ TEM. ACS Applied Materials & Interfaces, 2016, 8, 32333-32340.	4.0	54
60	Hydrolysis of a two-membered silica ring on the amorphous silica surface. Journal of Chemical Physics, 2004, 120, 1044-1054.	1.2	53
61	Flat bands in the CoSn-type compounds. Physical Review B, 2020, 102, .	1.1	52
62	Tuning magnetic order in the van der Waals metal <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Fe</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:r by cobalt substitution. Physical Review Materials, 2020, 4, .	2.4	52
63	Discrete Electronic Bands in Semiconductors and Insulators: Potential High-Light-Yield Scintillators. Physical Review Applied, 2015, 3, .	1.5	51
64	Photo-Oxidation of Polyhydroxyl Molecules onTiO2Surfaces: From Hole Scavenging to Light-Induced Self-Assembly ofTiO2-Cyclodextrin Wires. Physical Review Letters, 2007, 98, 066102.	2.9	50
65	Native defects and oxygen and hydrogen-related defect complexes in CdTe: Density functional calculations. Journal of Applied Physics, 2008, 104, 093521.	1.1	50
66	Compositionâ€Dependent Photoluminescence Properties and Antiâ€Counterfeiting Applications of A₂AgX₃ (AÂ=ÂRb, Cs; XÂ= ÂCl, Br, I). Advanced Functional Materials, 2021, 31, 2104941.	7.8	50
67	Crystal Synthesis and Frustrated Magnetism in Triangular Lattice CsRESe₂ (RE = Laâ€“Lu): Quantum Spin Liquid Candidates CsCeSe₂ and CsYbSe₂. , 2020, 2, 71-75.		49
68	Zero-Dimensional Hybrid Organicâ€“Inorganic Indium Bromide with Blue Emission. Inorganic Chemistry, 2021, 60, 1045-1054.	1.9	48
69	Potential thermoelectric performance of hole-doped Cu₂O. New Journal of Physics, 2013, 15, 043029.	1.2	47
70	Deciphering the effect of traps on electronic charge transport properties of methylammonium lead tribromide perovskite. Science Advances, 2020, 6, .	4.7	47
71	Predicting the thermodynamic stability of double-perovskite halides from density functional theory. APL Materials, 2018, 6, .	2.2	42
72	Antisite Pairs Suppress the Thermal Conductivity of BAs. Physical Review Letters, 2018, 121, 105901.	2.9	41

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73	Electron-phonon superconductivity in LaNiPO. Physical Review B, 2008, 78, .	1.1	40
74	Enhanced Born charges in III-VII,<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>IV-VII</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:m and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>V-VII</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:ms Physical Review B, 2010, 82, .	1.1	40
75	Native defects in antiferromagnetic topological insulator <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>MnBi</mml:mi><mml:mn>2</mml:mn></ Physical Review Materials, 2020, 4, .	0.9	40
76	Stabilization mechanisms of polar surfaces: ZnO surfaces. Physical Review B, 2008, 78, .	1.1	37
77	Prospective high thermoelectric performance of the heavily <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi mathvariant="bold-italic">p</mml:mi></mml:math> -doped half-Heusler compound CoVSn. Physical Review B, 2017, 95, .	1.1	37
78	First-principles study of native defects in TlBr: Carrier trapping, compensation, and polarization phemomenon. Journal of Applied Physics, 2010, 108, .	1.1	36
79	Bistability-Mediated Carrier Recombination at Light-Induced Boron-Oxygen Complexes in Silicon. Physical Review Letters, 2006, 97, 256602.	2.9	35
80	Mn4+ emission in pyrochlore oxides. Journal of Luminescence, 2015, 157, 69-73.	1.5	35
81	Rb₄Ag₂BiBr₉: A Lead-Free Visible Light Absorbing Halide Semiconductor with Improved Stability. Inorganic Chemistry, 2019, 58, 4446-4455.	1.9	35
82	Crystal growth and scintillation properties of pure and Tl-doped Cs3Cu2I5. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2021, 991, 164963.	0.7	35
83	Properties of alkaline-earth-filled skutterudite antimonides:<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"		

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91	Manipulation of fullerene-induced impurity states in carbon peapods. Physical Review B, 2003, 68, .	1.1	25
92	DXcenters in GaAs and GaSb. Physical Review B, 2005, 72, .	1.1	25
93	Transport and optical properties of heavily hole-doped semiconductors BaCu2Se2 and BaCu2Te2. Journal of Solid State Chemistry, 2011, 184, 2744-2750.	1.4	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.	6.6	24
95	Determination of miscibility in MgO-ZnO nanocrystal alloys by x-ray absorption spectroscopy. Applied Physics Letters, 2011, 99, 261901.	1.5	23
96	Microscopic origin of multiple exciton emission in low-dimensional lead halide perovskites. Journal of Chemical Physics, 2019, 151, 181101.	1.2	23
97	Electronic structure engineering of elpasolites: Case of Cs2AgYCl6. Journal of Luminescence, 2013, 143, 710-714.	1.5	22
98	Scintillation Properties and Electronic Structures of the Intrinsic and Extrinsic Mixed Elpasolites<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Cs</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub><mml:mrow><mml:mi mathvariant="normal">I</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></m. Physical Review Applied, 2019, 12, .	1.5	22
99	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>Sb<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow	1.1	21
100	Intense deep-red zero phonon line emission of Mn⁴⁺ in double perovskite La₄Ti₃O₁₂. Physical Chemistry Chemical Physics, 2019, 21, 25108-25117.	1.3	21
101	AX centers in II-VI semiconductors: Hybrid functional calculations. Applied Physics Letters, 2011, 98, .	1.5	18
102	First principles study of native defects in InI. Journal of Applied Physics, 2011, 109, 113518.	1.1	17
103	Transparent interface between classical molecular dynamics and first-principles molecular dynamics. International Journal of Quantum Chemistry, 2003, 93, 1-8.	1.0	16
104	Chemical Trend of Transition-Metal Doping in WSe2. Physical Review Applied, 2019, 12, .	1.5	16
105	Hydrogen in anion vacancies of semiconductors. Physical Review B, 2009, 79, .	1.1	15
106	Direct Evidence of Excitonâ€“Exciton Annihilation in Single-Crystalline Organic Metal Halide Nanotube Assemblies. Journal of Physical Chemistry Letters, 2018, 9, 2164-2169.	2.1	15
107	(CH 3 NH 3)AuX 4 â‹…H 2 O (X=Cl, Br) and (CH 3 NH 3)AuCl 4 : Lowâ€Band Gap Leadâ€Free Layered Gold Halide Perovskite Materials. Chemistry - A European Journal, 2019, 25, 9875-9884.	1.7	15
108	Excitation Energies of Localized Correlated Defects via Quantum Monte Carlo: A Case Study of Mn⁴⁺-Doped Phosphors. Journal of Physical Chemistry Letters, 2019, 10, 67-74.	2.1	15

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109	Robust Ferromagnetism in Highly Strained <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>SrCoO</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn> Thin Films. Physical Review X, 2020, 10, .	2.8	15
110	Adsorption-controlled growth of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>MnTe</mml:mi><mml:msub><mml:mrow><mml:mo>(</mml:mo> by molecular beam epitaxy exhibiting stoichiometry-controlled magnetism. Physical Review Materials, 2020, 4, .	0.9	15
111	Electronic structure, magnetism and superconductivity of layered iron compounds. Physica C: Superconductivity and Its Applications, 2009, 469, 886-889.	0.6	14
112	Crystal structure, electronic structure, temperature-dependent optical and scintillation properties of CsCe₂Br₇. Journal of Materials Chemistry C, 2015, 3, 11366-11376.	2.7	14
113	(NH₄)₂AgX₃ (X = Br, I): 1D Silver Halides with Broadband White Light Emission and Improved Stability. ACS Materials Au, 2021, 1, 62-68.	2.6	14
114	Tuning the room temperature ferromagnetism in Fe₅GeTe₂ by arsenic substitution. 2D Materials, 2022, 9, 015013.	2.0	14
115	Hydrogen-Mediated Nitrogen Clustering in Dilute III-V Nitrides. Physical Review Letters, 2006, 97, 075503.	2.9	13
116	Bismuth-induced deep levels and carrier compensation in CdTe. Physical Review B, 2008, 78, .	1.1	13
117	First-principles study of back-contact effects on CdTe thin-film solar cells. Physical Review B, 2009, 80, .	1.1	13
118	Topological defects and the Staebler-Wronski effect in hydrogenated amorphous silicon. Applied Physics Letters, 2005, 87, 191903.	1.5	12
119	Crystal structure, electronic structure, optical and scintillation properties of self-activated Cs4YbI6. Journal of Luminescence, 2018, 201, 460-465.	1.5	12
120	Quantum, classical, and multi-scale simulation of silicaâ€“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, .	1.1	11
122	Vibrational signatures of OTe and OTeâ€“VCd in CdTe: A first-principles study. Computational Materials Science, 2010, 49, S242-S245.	1.4	11
123	Electronic structure, small polaron, and F center in LiCaAlF6. Journal of Applied Physics, 2012, 112, 123516.	1.1	11
124	Zero-dimensional metal oxide Li4TiO4. Journal of Materials Chemistry C, 2019, 7, 5710-5715.	2.7	11
125	Additive-assisted synthesis and optoelectronic properties of (CH3NH3)4Bi6I22. Inorganic Chemistry Frontiers, 2020, 7, 1564-1572.	3.0	11
126	Crystal growth, density functional theory, and scintillation properties of Tl3LnCl6:Ce3+ and TlLn2Cl7:Ce3+ (Ln = Y, Gd). Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2021, 995, 165047.	0.7	11

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127	(C₇H₁₁N₂)₂MBr₄ (M=Cu, Zn): Xâ€Ray Sensitive 0D Hybrid Metal Halides with Tunable Broadband Emission. European Journal of Inorganic Chemistry, 2022, 2022, e202100954.	1.0	11
128	DX centers in CdTe: A density functional study. Applied Physics Letters, 2008, 92, 181908.	1.5	10
129	Optoelectronic properties of candidate photovoltaic Cu2PbSiS4, Ag2PbGeS4 and KAg2SbS4 semiconductors. Journal of Alloys and Compounds, 2018, 746, 405-412.	2.8	10
130	Synthesis, crystal and electronic structures and optical properties of (HIm)2Hg3Cl8 and (HIm)HgI3 (HIm = imidazolium). Journal of Solid State Chemistry, 2018, 258, 551-558.	1.4	10
131	Doping Y₂O₃ with Mn⁴⁺ for energy-efficient lighting. Journal of Materials Chemistry C, 2018, 6, 4171-4176.	2.7	10
132	First principles study of O defects in CdSe. Physica B: Condensed Matter, 2012, 407, 2841-2845.	1.3	9
133	Ternary chalcogenides<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">C</mml:mi><mml:msub><mml:mi mathvariant="normal">s</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">Z</mml:mi><mml:msub><mml:mi mathvariant="normal">n</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mi mathvariant="normal">	1.1	9
134	Impurity-induced deep centers in Tl6SI4. Journal of Applied Physics, 2017, 121, 145102.	1.1	9
135	Thallium-based scintillators for high-resolution gamma-ray spectroscopy: Ce<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e576" altimg="si37.svg"><mml:msup><mml:mrow /><mml:mrow><mml:mn>3</mml:mn><mml:mo>+</mml:mo></mml:mrow></mml:msup></mml:math>-doped Tl2LaCl5 and Tl2LaBr<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"	0.7	9
136	Intrinsic and complex defect engineering of quasi-one-dimensional ribbons <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Sb</mml:mi><mml:mn>2</mml:mn></mml: mathvariant="normal">S</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> for photovoltaics performance. Physical Review Materials, 2021, 5, .	0.9	9
137	Effects of impurity doping on ionic conductivity and polarization phenomenon in TlBr. Applied Physics Letters, 2013, 102, 082102.	1.5	8
138	Electronic shell structures, self-trapped excitons, and defect-bound excitons in Li₂B₁₂H₁₂. Journal of Materials Chemistry C, 2019, 7, 14342-14349.	2.7	8
139	Role of Lithium Codoping in Enhancing the Scintillation Yield of Aluminate Garnets. Physical Review Applied, 2020, 13, .	1.5	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.	2.1	8
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142	Native defects in Tl6SI4: Density functional calculations. Journal of Applied Physics, 2015, 117, .	1.1	7
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