

Mao-Hua Du

List of Publications by Year in descending order

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169
papers

10,636
citations

28274

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34986

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176
all docs

176
docs citations

176
times ranked

11702
citing authors

#	ARTICLE	IF	CITATIONS
1	Tuning the room temperature ferromagnetism in Fe_5GeTe_2 by arsenic substitution. <i>2D Materials</i> , 2022, 9, 015013.	4.4	14
2	$(\text{C}_7\text{H}_{11}\text{N}_2)_2\text{MBr}_4$ (M=Cu, Zn): X-Ray Sensitive OD Hybrid Metal Halides with Tunable Broadband Emission. <i>European Journal of Inorganic Chemistry</i> , 2022, 2022, e202100954.	2.0	11
3	Crystal growth, density functional theory, and scintillation properties of TiMgX_3 (X=Cl, Br, I). <i>Chemical Physics</i> , 2022, 558, 111535.	1.9	2
4	Surface-Driven Evolution of the Anomalous Hall Effect in Magnetic Topological Insulator MnBi_2Te_4 Thin Films. <i>Advanced Functional Materials</i> , 2022, 32, .	14.9	2
5	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
6	$\text{TiSr}_2\text{Ti}_5\text{Eu}_2$: A new high density scintillator for gamma-ray detection. <i>Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment</i> , 2021, 988, 164876.	1.6	7
7	Crystal growth and scintillation properties of pure and Tl-doped $\text{Cs}_3\text{Cu}_2\text{I}_5$. <i>Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment</i> , 2021, 991, 164963.	1.6	35
8	Zero-Dimensional Hybrid Organic-Inorganic Indium Bromide with Blue Emission. <i>Inorganic Chemistry</i> , 2021, 60, 1045-1054.	4.0	48
9	Crystal growth, density functional theory, and scintillation properties of $\text{Ti}_3\text{LnCl}_6\text{:Ce}^{3+}$ and $\text{TiLn}_2\text{Cl}_7\text{:Ce}^{3+}$ (Ln = Y, Gd). <i>Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment</i> , 2021, 995, 165047.	1.6	11
10	Intrinsic and complex defect engineering of quasi-one-dimensional ribbons Sb_2S_3 for photovoltaics performance. <i>Physical Review Materials</i> , 2021, 5, .	2.4	9
11	Hierarchical excitations from correlated spin tetrahedra on the breathing pyrochlore lattice. <i>Physical Review B</i> , 2021, 103, .	3.2	5
12	$(\text{NH}_4)_2\text{AgX}_3$ (X = Br, I): 1D Silver Halides with Broadband White Light Emission and Improved Stability. <i>ACS Materials Au</i> , 2021, 1, 62-68.	6.0	14
13	Magnetic properties of the Shastry-Sutherland lattice material BaNd_2F_8 . <i>Physical Review Materials</i> , 2021, 5, .		
14	Design of High-Performance Lead-Free Quaternary Antiperovskites for Photovoltaics via Ion Type Inversion and Anion Ordering. <i>Journal of the American Chemical Society</i> , 2021, 143, 12369-12379.	13.7	24
15	Metal Halide Scaffolded Assemblies of Organic Molecules with Enhanced Emission and Room Temperature Phosphorescence. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 8229-8236.	4.6	27
16	Role of Polycyclic Aromatic Alkylammonium Cations in Tuning the Electronic Properties and Band Alignment of Two-Dimensional Hybrid Perovskite Semiconductors. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 9754-9760.	4.6	8
17	Composition-Dependent Photoluminescence Properties and Anti-Counterfeiting Applications of AA_2AgX_3 (AA=Arb, Cs; X=Cl, Br, I). <i>Advanced Functional Materials</i> , 2021, 31, 2104941.	14.9	50
18	Photophysical properties of zero-dimensional perovskites studied by PBE0 and GW+BSE methods. <i>Journal of Applied Physics</i> , 2021, 130, 203106.	2.5	4

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19	Rb ₂ CuX 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
20	Emission Trend of Multiple Self-Trapped Excitons in Luminescent 1D Copper Halides. <i>ACS Energy Letters</i> , 2020, 5, 464-469.	17.4	111
21	Crystal Synthesis and Frustrated Magnetism in Triangular Lattice Cs ₂ RE ₂ Se ₂ (RE = La, Lu): Quantum Spin Liquid Candidates CsCeSe ₂ and CsYbSe ₂ . <i>ACS Energy Letters</i> , 2020, 2, 71-75.		49
22	(INVITED) First-principles calculations of quantum transitions at local centers. <i>Optical Materials: X</i> , 2020, 8, 100066.	0.8	5
23	Reaching 90% Photoluminescence Quantum Yield in One-Dimensional Metal Halide C ₄ N ₂ H ₁₄ PbBr ₄ by Pressure-Suppressed Nonradiative Loss. <i>Journal of the American Chemical Society</i> , 2020, 142, 16001-16006.	13.7	109
24	Flat bands in the CoSn-type compounds. <i>Physical Review B</i> , 2020, 102, .	3.2	52
25	Deciphering the effect of traps on electronic charge transport properties of methylammonium lead tribromide perovskite. <i>Science Advances</i> , 2020, 6, .	10.3	47
26	OD and 2D: The Cases of Phenylethylammonium Tin Bromide Hybrids. <i>Chemistry of Materials</i> , 2020, 32, 4692-4698.	6.7	72
27	Robust Ferromagnetism in Highly Strained SrCoO ₃ Thin Films. <i>Physical Review X</i> , 2020, 10, .	8.9	15
28	K ₂ CuX 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	Role of Lithium Codoping in Enhancing the Scintillation Yield of Aluminate Garnets. <i>Physical Review Applied</i> , 2020, 13, .	3.8	8
30	Thallium-based scintillators for high-resolution gamma-ray spectroscopy: Ce-doped Tl ₂ LaCl ₅ and Tl ₂ LaBr ₅ . <i>Physical Review Applied</i> , 2020, 13, .	1.6	9
31	Additive-assisted synthesis and optoelectronic properties of (CH ₃ NH ₃) ₄ Bi ₆ I ₂₂ . <i>Inorganic Chemistry Frontiers</i> , 2020, 7, 1564-1572.	6.0	11
32	Density functional studies of defects and defect-related luminescence in Mg ₃ N ₂ . <i>Physical Review Materials</i> , 2020, 4, .	2.4	2
33	Tuning magnetic order in the van der Waals metal Fe ₂ Te ₅ by cobalt substitution. <i>Physical Review Materials</i> , 2020, 4, .	2.4	15
34	Adsorption-controlled growth of MnTe by molecular beam epitaxy exhibiting stoichiometry-controlled magnetism. <i>Physical Review Materials</i> , 2020, 4, .	2.4	15
35	Native defects in antiferromagnetic topological insulator MnBi ₂ Te ₄ . <i>Physical Review Materials</i> , 2020, 4, .	2.4	15
36	Atomic-Scale Study of Intrinsic Defects Suppressing the Thermal Conductivity of Boron Arsenide. <i>Microscopy and Microanalysis</i> , 2019, 25, 942-943.	0.4	0

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37	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
38	Frontispiece: $(\text{CH}_3\text{NH}_3)_2\text{AuX}_4 \cdot \text{H}_2\text{O}$ (X=Cl, Br) and $(\text{CH}_3\text{NH}_3)_4\text{AuCl}_4$: Low-Band Gap Lead-Free Layered Gold Halide Perovskite Materials. <i>Chemistry - A European Journal</i> , 2019, 25, .	3.3	0
39	Bulk Assembly of Zero-Dimensional Organic Lead Bromide Hybrid with Efficient Blue Emission. , 2019, 1, 594-598.		92
40	Bright Luminescence from Nontoxic CsCu_2X_3 (X = Cl, Br, I). , 2019, 1, 459-465.		148
41	Chemical Trend of Transition-Metal Doping in WSe_2 . <i>Physical Review Applied</i> , 2019, 12, .	3.8	16
42	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
43	$(\text{CH}_3\text{NH}_3)_2\text{AuX}_4 \cdot \text{H}_2\text{O}$ (X=Cl, Br) and $(\text{CH}_3\text{NH}_3)_4\text{AuCl}_4$: Low-Band Gap Lead-Free Layered Gold Halide Perovskite Materials. <i>Chemistry - A European Journal</i> , 2019, 25, 9875-9884.	3.3	15
44	Zero-dimensional metal oxide Li_4TiO_4 . <i>Journal of Materials Chemistry C</i> , 2019, 7, 5710-5715.	5.5	11
45	Near-Unity Photoluminescence Quantum Yield in Blue-Emitting $\text{Cs}_3\text{Cu}_2\text{Br}_5$ ($0 \leq x \leq 5$). <i>ACS Applied Electronic Materials</i> , 2019, 1, 269-274.	4.3	184
46	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
47	$\text{Rb}_4\text{Ag}_2\text{BiBr}_9$: A Lead-Free Visible Light Absorbing Halide Semiconductor with Improved Stability. <i>Inorganic Chemistry</i> , 2019, 58, 4446-4455.	4.0	35
48	Microscopic origin of multiple exciton emission in low-dimensional lead halide perovskites. <i>Journal of Chemical Physics</i> , 2019, 151, 181101.	3.0	23
49	Electronic shell structures, self-trapped excitons, and defect-bound excitons in $\text{Li}_2\text{B}_{12}\text{H}_{12}$. <i>Journal of Materials Chemistry C</i> , 2019, 7, 14342-14349.	5.5	8
50	Low dimensional metal halide perovskites and hybrids. <i>Materials Science and Engineering Reports</i> , 2019, 137, 38-65.	31.8	300
51	Excitation Energies of Localized Correlated Defects via Quantum Monte Carlo: A Case Study of Mn^{4+} -Doped Phosphors. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 67-74.	4.6	15
52	Bulk Assembly of Corrugated 1D Metal Halides with Broadband Yellow Emission. <i>Advanced Optical Materials</i> , 2019, 7, 1801474.	7.3	65
53	Intense deep-red zero phonon line emission of Mn^{4+} in double perovskite $\text{La}_4\text{Ti}_3\text{O}_{12}$. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 25108-25117.	2.8	21
54	Impact of metal lone pair on luminescence quantum efficiency in low-dimensional halide perovskites. <i>Physical Review Materials</i> , 2019, 3, .	2.4	60

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55	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

56 Tuning the Magnetic Properties and Structural Stabilities of the 2-17-3 Magnets<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"

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109	Effects of impurity doping on ionic conductivity and polarization phenomenon in TlBr. Applied Physics Letters, 2013, 102, 082102.	3.3	8
110	Potential thermoelectric performance of hole-doped Cu_2O . New Journal of Physics, 2013, 15, 043029.	2.9	47
111	High magnetocrystalline anisotropy in oxides with near cubic local environments. Applied Physics Letters, 2013, 102, .	3.3	6
112	Resistivity, carrier trapping, and polarization phenomenon in semiconductor radiation detection materials. Proceedings of SPIE, 2012, , .	0.8	6
113	Electronic structure, energy transport, and optical properties of halide scintillators. Proceedings of SPIE, 2012, , .	0.8	4
114	Energy transport and scintillation of cerium-doped elpasolite $\text{Cs}_2\text{LiYCl}_6$: Hybrid density functional calculations. Physical Review B, 2012, 86, .	3.2	78
115	Electronic structure, small polaron, and F center in LiCaAlF_6 . Journal of Applied Physics, 2012, 112, 123516.	2.5	11
116	First-principles study of impurities in TlBr. Journal of Applied Physics, 2012, 111, 073519.	2.5	5
117	Electronic structure and defect properties of Tl_2Se : Density functional calculations. Physical Review B, 2012, 86, .	3.2	28
118	First principles study of O defects in CdSe. Physica B: Condensed Matter, 2012, 407, 2841-2845.	2.7	9
119	What causes high resistivity in CdTe. New Journal of Physics, 2012, 14, 063020.	2.9	57
120	Doping dependence of thermoelectric performance in MoSb_3 . Physical Review Letters, 2011, 107, 207207.	3.2	21
121	Determination of miscibility in MgO-ZnO nanocrystal alloys by x-ray absorption spectroscopy. Applied Physics Letters, 2011, 99, 261901.	3.3	23
122	Spin Ice: Magnetic Excitations without Monopole Signatures Using Muon Spin Rotation. Physical Review Letters, 2011, 107, 207207.	7.8	60
123	Transport and optical properties of heavily hole-doped semiconductors BaCu_2Se_2 and BaCu_2Te_2 . Journal of Solid State Chemistry, 2011, 184, 2744-2750.	2.9	25
124	Giant anharmonic phonon scattering in PbTe. Nature Materials, 2011, 10, 614-619.	27.5	561
125	Anionic and Hidden Hydrogen in ZnO. Physical Review Letters, 2011, 106, 115502.	7.8	84
126	First principles study of native defects in InI. Journal of Applied Physics, 2011, 109, 113518.	2.5	17

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145	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
146	Bismuth-induced deep levels and carrier compensation in CdTe. <i>Physical Review B</i> , 2008, 78, .	3.2	13
147	Trapped-Dopant Model of Doping in Semiconductor Nanocrystals. <i>Nano Letters</i> , 2008, 8, 2878-2882.	9.1	69
148	Electronic Structure, Magnetism and Spin-Fluctuations in Fe-As Based Superconductors. <i>Materials Research Society Symposia Proceedings</i> , 2008, 1148, 1.	0.1	0
149	Stabilization mechanisms of polar surfaces: ZnO surfaces. <i>Physical Review B</i> , 2008, 78, .	3.2	37
150	DX centers in CdTe: A density functional study. <i>Applied Physics Letters</i> , 2008, 92, 181908.	3.3	10
151	Carrier compensation in semi-insulating CdTe: First-principles calculations. <i>Physical Review B</i> , 2008, 77, .	3.2	59
152	Photo-Oxidation of Polyhydroxyl Molecules onTiO ₂ Surfaces: From Hole Scavenging to Light-Induced Self-Assembly ofTiO ₂ -Cyclodextrin Wires. <i>Physical Review Letters</i> , 2007, 98, 066102.	7.8	50
153	Unifying Chemical Bonding Models for Boranes. <i>Materials Research Society Symposia Proceedings</i> , 2007, 1038, 1.	0.1	1
154	First-principles study of native defects in anataseTiO ₂ . <i>Physical Review B</i> , 2006, 73, .	3.2	346
155	Bistability-Mediated Carrier Recombination at Light-Induced Boron-Oxygen Complexes in Silicon. <i>Physical Review Letters</i> , 2006, 97, 256602.	7.8	35
156	Ion relaxation and hydrogen LVM in H-irradiated GaAsN. <i>Physica B: Condensed Matter</i> , 2006, 376-377, 583-586.	2.7	2
157	Quantum, classical, and multi-scale simulation of silica-water interaction: molecules, clusters, and extended systems. <i>Journal of Computer-Aided Materials Design</i> , 2006, 13, 161-183.	0.7	11
158	Hydrogen-Mediated Nitrogen Clustering in Dilute III-V Nitrides. <i>Physical Review Letters</i> , 2006, 97, 075503.	7.8	13
159	Hydrogen pairs and local vibrational frequencies in H-irradiatedGaAs1-yNy. <i>Physical Review B</i> , 2005, 72, .	3.2	33
160	Topological defects and the Staebler-Wronski effect in hydrogenated amorphous silicon. <i>Applied Physics Letters</i> , 2005, 87, 191903.	3.3	12
161	DXcenters in GaAs and GaSb. <i>Physical Review B</i> , 2005, 72, .	3.2	25
162	First-Principles Prediction of Icosahedral Quantum Dots for Tetravalent Semiconductors. <i>Physical Review Letters</i> , 2004, 93, .	7.8	55

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163	Hydrolysis of a two-membered silica ring on the amorphous silica surface. Journal of Chemical Physics, 2004, 120, 1044-1054.	3.0	53
164	Coherent Electron Transport through an Azobenzene Molecule: A Light-Driven Molecular Switch. Physical Review Letters, 2004, 92, 158301.	7.8	249
165	Transparent interface between classical molecular dynamics and first-principles molecular dynamics. International Journal of Quantum Chemistry, 2003, 93, 1-8.	2.0	16
166	Bulk Separative Enrichment in Metallic or Semiconducting Single-Walled Carbon Nanotubes. Nano Letters, 2003, 3, 1245-1249.	9.1	246
167	Water-silica surface interactions: A combined quantum-classical molecular dynamic study of energetics and reaction pathways. Journal of Chemical Physics, 2003, 119, 6418-6422.	3.0	78
168	Manipulation of fullerene-induced impurity states in carbon peapods. Physical Review B, 2003, 68, .	3.2	25
169	Crossover in energy redistribution during C60@Xe144 surface impact. Physical Review B, 2001, 64, .	3.2	1