Hongliang Shi

List of Publications by Year in Descending Order

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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.

68 papers	3,160 citations	28 h-index	55 g-index
68 ext. papers	3,611 ext. citations	4.1 avg, IF	5.57 L-index

#	Paper	IF	Citations
68	Photophysical properties of zero-dimensional perovskites studied by PBE0 and GW+BSE methods. *Journal of Applied Physics*, **2021**, 130, 203106	2.5	1
67	Intrinsic and complex defect engineering of quasi-one-dimensional ribbons Sb2S3 for photovoltaics performance. *Physical Review Materials*, **2021**, 5,	3.2	1
66	Strain-enhanced power conversion efficiency of a BP/SnSe van der Waals heterostructure. *Physical Chemistry Chemical Physics*, **2020**, 22, 14787-14795	3.6	7
65	Density functional studies of defects and defect-related luminescence in Mg3N2. *Physical Review Materials*, **2020**, 4,	3.2	1
64	Competitive conductive mechanism of interstitial Ag and oxygen vacancies in Ag/Ta2O5/Pt stack. *Journal of Applied Physics*, **2019**, 126, 065104	2.5	1
63	Modulation of resistive switching in Pt/LiCoO2/SiO2/Si stacks. *Journal of Materials Science: Materials in Electronics*, **2019**, 30, 4753-4759	2.1	2
62	Stability and Repeatability of a Karst-like Hierarchical Porous Silicon Oxide-Based Memristor. *ACS Applied Materials & Interfaces*, **2019**, 11, 21734-21740	9.5	8
61	Lithium ion trapping mechanism of SiO in LiCoO based memristors. *Scientific Reports*, **2019**, 9, 5081	4.9	9
60	Near-Unity Photoluminescence Quantum Yield in Blue-Emitting Cs3Cu2Br5−xIx (0 ≤ x ≤ 5). *ACS Applied Electronic Materials*, **2019**, 1, 269-274	4	124
59	Impact of metal ns2 lone pair on luminescence quantum efficiency in low-dimensional halide perovskites. *Physical Review Materials*, **2019**, 3,	3.2	40
58	Electronic shell structures, self-trapped excitons, and defect-bound excitons in Li2B12H12. *Journal of Materials Chemistry C*, **2019**, 7, 14342-14349	7.1	2
57	Barrier Reduction of Lithium Ion Tunneling through Graphene with Hybrid Defects: First-Principles Calculations. *Advanced Theory and Simulations*, **2018**, 1, 1700009	3.5	7
56	A Zero-Dimensional Organic Seesaw-Shaped Tin Bromide with Highly Efficient Strongly Stokes-Shifted Deep-Red Emission. *Angewandte Chemie*, **2018**, 130, 1033-1036	3.6	44
55	Doping Y2O3 with Mn4+ for energy-efficient lighting. *Journal of Materials Chemistry C*, **2018**, 6, 4171-4176	7.1	8
54	Zero-dimensional Cs4EuX6 (X = Br, I) all-inorganic perovskite single crystals for gamma-ray spectroscopy. *Journal of Materials Chemistry C*, **2018**, 6, 6647-6655	7.1	40
53	A Zero-Dimensional Organic Seesaw-Shaped Tin Bromide with Highly Efficient Strongly Stokes-Shifted Deep-Red Emission. *Angewandte Chemie - International Edition*, **2018**, 57, 1021-1024	16.4	152
52	Tunable band offsets in the BP/PO van der Waals heterostructure: first-principles calculations. *Physical Chemistry Chemical Physics*, **2018**, 20, 29931-29938	3.6	5

51	Broadband Emission in Hybrid Organic-Inorganic Halides of Group 12 Metals. *ACS Omega*, **2018**, 3, 18791-18802	3.9	47
50	Crystal structure, electronic structure, optical and scintillation properties of self-activated Cs4YbI6. *Journal of Luminescence*, **2018**, 201, 460-465	3.8	8
49	Unraveling luminescence mechanisms in zero-dimensional halide perovskites. *Journal of Materials Chemistry C*, **2018**, 6, 6398-6405	7.1	110
48	Impurity-induced deep centers in Tl6SI4. *Journal of Applied Physics*, **2017**, 121, 145102	2.5	9
47	Prospective high thermoelectric performance of the heavily p-doped half-Heusler compound CoVSn. *Physical Review B*, **2017**, 95,	3.3	26
46	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	13	98
45	Bismuth chalcohalides and oxyhalides as optoelectronic materials. *Physical Review B*, **2016**, 93,	3.3	56
44	Scintillation Properties and Electronic Structures of the Intrinsic and Extrinsic Mixed Elpasolites Cs2NaRBr3I3 (R=La, Y). *Physical Review Applied*, **2016**, 5,	4.3	18
43	Fast Diffusion of Native Defects and Impurities in Perovskite Solar Cell Material CH3NH3PbI3. *Chemistry of Materials*, **2016**, 28, 4349-4357	9.6	112
42	Native defects in Tl6SI4: Density functional calculations. *Journal of Applied Physics*, **2015**, 117, 175701	2.5	7
41	Ba2TeO as an optoelectronic material: First-principles study. *Journal of Applied Physics*, **2015**, 117, 195705	2.5	3
40	Mesoporous MnCeOx solid solutions for low temperature and selective oxidation of hydrocarbons. *Nature Communications*, **2015**, 6, 8446	17.4	175
39	Crystal structure, electronic structure, temperature-dependent optical and scintillation properties of CsCe2Br7. *Journal of Materials Chemistry C*, **2015**, 3, 11366-11376	7.1	12
38	Discrete Electronic Bands in Semiconductors and Insulators: Potential High-Light-Yield Scintillators. *Physical Review Applied*, **2015**, 3,	4.3	37
37	Magnetism in Na-filled Fe-based skutterudites. *Scientific Reports*, **2015**, 5, 10782	4.9	9
36	Electronic, transport, and optical properties of bulk and mono-layer PdSe2. *Applied Physics Letters*, **2015**, 107, 153902	3.4	124
35	Li2Se:Te as a neutron scintillator. *Journal of Alloys and Compounds*, **2015**, 647, 906-910	5.7	7
34	Connecting Thermoelectric Performance and Topological-Insulator Behavior: Bi2Te3 and Bi2Te2Se from First Principles. *Physical Review Applied*, **2015**, 3,	4.3	140

33	Nanoscale Transition Metal Dichalcogenides: Structures, Properties, and Applications. *Critical Reviews in Solid State and Materials Sciences*, **2014**, 39, 319-367	10.1	106
32	Shallow halogen vacancies in halide optoelectronic materials. *Physical Review B*, **2014**, 90,	3.3	98
31	Ternary chalcogenides Cs2Zn3Se4 and Cs2Zn3Te4: Potential p-type transparent conducting materials. *Physical Review B*, **2014**, 90,	3.3	8
30	Phase transition and band-structure tuning in InN through uniaxial and biaxial strains. *Journal of Physics Condensed Matter*, **2014**, 26, 025501	1.8	10
29	Comparing the effects of uniaxial and biaxial strains on the structural stability and electronic structure in wurtzite ZnS. *Journal of Applied Physics*, **2013**, 114, 023514	2.5	6
28	Quasiparticle band structures and optical properties of strained monolayer MoS2 and WS2. *Physical Review B*, **2013**, 87,	3.3	662
27	Hybrid density functional theory studies of AlN and GaN under uniaxial strain. *Journal of Physics Condensed Matter*, **2013**, 25, 045801	1.8	17
26	Strong ferromagnetism in hydrogenated monolayer MoS2 tuned by strain. *Physical Review B*, **2013**, 88,	3.3	113
25	First-principles study of □Pu2O3. *Journal of Nuclear Materials*, **2012**, 420, 159-163	3.3	17
24	Electronic and Magnetic Properties of Graphene/Fluorographene Superlattices. *Journal of Physical Chemistry C*, **2012**, 116, 18278-18283	3.8	24
23	Hybrid density functional theory study of band gap tuning in AlN and GaN through equibiaxial strains. *Applied Physics Letters*, **2012**, 100, 022104	3.4	32
22	Electron band structure of the high pressure cubic phase of AlH3. *Journal of Physics: Conference Series*, **2012**, 377, 012093	0.3	6
21	Magnetic behavior of Fe(Se,Te) systems: First-principles calculations. *Journal of Applied Physics*, **2011**, 110, 043917	2.5	23
20	Structural, electronic, mechanical, and thermodynamic properties of UN2: Systematic density functional calculations. *Journal of Nuclear Materials*, **2011**, 410, 46-51	3.3	21
19	Magnetic coupling properties of Mn-doped AlN nanowires: First-principles calculations. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2011**, 375, 1686-1689	2.3	10
18	Anomalous structural transformation, spontaneous polarization, piezoelectric response, and band structure of semiconductor aluminum nitride under hydrostatic pressure. *Journal of Applied Physics*, **2011**, 110, 103712	2.5	14
17	First-principles LDA+U and GGA+U study of neptunium dioxide. *Physical Review B*, **2010**, 81,	3.3	52
16	Mechanical and chemical bonding properties of ground state BeH2. *European Physical Journal B*, **2010**, 74, 303-308	1.2	20

15	Electronic structure and magnetic coupling properties of Gd-doped AlN: first-principles calculations. *European Physical Journal B*, **2010**, 77, 345-349	1.2	7
14	Structural, mechanical, thermodynamic, and electronic properties of thorium hydrides from first-principles. *Journal of Nuclear Materials*, **2010**, 401, 124-129	3.3	19
13	Structural, electronic, and thermodynamic properties of UN: Systematic density functional calculations. *Journal of Nuclear Materials*, **2010**, 406, 218-222	3.3	29
12	Anomalous optical and electronic properties of dense sodium. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2010**, 374, 4458-4464	2.3	
11	First-principles study of UC2 and U2C3. *Journal of Nuclear Materials*, **2010**, 396, 218-222	3.3	18
10	First-principles study of ground-state properties and high pressure behavior of ThO2. *Journal of Nuclear Materials*, **2010**, 399, 181-188	3.3	54
9	Optical properties of UO2 and PuO2. *Journal of Nuclear Materials*, **2010**, 400, 151-156	3.3	60
8	First-Principles Study of Magnetic Properties of 3d Transition Metals Doped in ZnO Nanowires. *Nanoscale Research Letters*, **2009**, 4, 480-484	5	43
7	Electronic structures and mechanical properties of uranium monocarbide from first-principles LDA+U and GGA+U calculations. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2009**, 373, 3577-3581	2.3	35
6	Magnetic coupling properties of rare-earth metals (Gd, Nd) doped ZnO: First-principles calculations. *Journal of Applied Physics*, **2009**, 106, 023910	2.5	72
5	Studies of tetragonal PbTiO3subjected to uniaxial stress along thec-axis. *Journal of Physics Condensed Matter*, **2008**, 20, 175210	1.8	20
4	Magnetic coupling properties of Mn-doped ZnO nanowires: First-principles calculations. *Journal of Applied Physics*, **2008**, 103, 073903	2.5	21
3	Elasticity, band structure, and piezoelectricity of BexZn1⊠O alloys. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2008**, 372, 2930-2933	2.3	34
2	p-type doping of GaInNAs quaternary alloys. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2008**, 373, 165-168	2.3	6
1	Band-gap bowing and p-type doping of (Zn, Mg, Be)O wide-gap semiconductor alloys: a first-principles study. *European Physical Journal B*, **2008**, 66, 439-444	1.2	53