

Hongliang Shi

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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	Quasiparticle band structures and optical properties of strained monolayer MoS ₂ and WS ₂ . <i>Physical Review B</i> , 2013 , 87,	3.3	662
67	Mesoporous MnCeO _x solid solutions for low temperature and selective oxidation of hydrocarbons. <i>Nature Communications</i> , 2015 , 6, 8446	17.4	175
66	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	16.4	152
65	Connecting Thermoelectric Performance and Topological-Insulator Behavior: Bi ₂ Te ₃ and Bi ₂ Te ₂ Se from First Principles. <i>Physical Review Applied</i> , 2015 , 3,	4.3	140
64	Near-Unity Photoluminescence Quantum Yield in Blue-Emitting Cs ₃ Cu ₂ Br ₅ I _x (0 ≤ x ≤ 5). <i>ACS Applied Electronic Materials</i> , 2019 , 1, 269-274	4	124
63	Electronic, transport, and optical properties of bulk and mono-layer PdSe ₂ . <i>Applied Physics Letters</i> , 2015 , 107, 153902	3.4	124
62	Strong ferromagnetism in hydrogenated monolayer MoS ₂ tuned by strain. <i>Physical Review B</i> , 2013 , 88,	3.3	113
61	Fast Diffusion of Native Defects and Impurities in Perovskite Solar Cell Material CH ₃ NH ₃ PbI ₃ . <i>Chemistry of Materials</i> , 2016 , 28, 4349-4357	9.6	112
60	Unraveling luminescence mechanisms in zero-dimensional halide perovskites. <i>Journal of Materials Chemistry C</i> , 2018 , 6, 6398-6405	7.1	110
59	Nanoscale Transition Metal Dichalcogenides: Structures, Properties, and Applications. <i>Critical Reviews in Solid State and Materials Sciences</i> , 2014 , 39, 319-367	10.1	106
58	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	13	98
57	Shallow halogen vacancies in halide optoelectronic materials. <i>Physical Review B</i> , 2014 , 90,	3.3	98
56	Magnetic coupling properties of rare-earth metals (Gd, Nd) doped ZnO: First-principles calculations. <i>Journal of Applied Physics</i> , 2009 , 106, 023910	2.5	72
55	Optical properties of UO ₂ and PuO ₂ . <i>Journal of Nuclear Materials</i> , 2010 , 400, 151-156	3.3	60
54	Bismuth chalcogenides and oxyhalides as optoelectronic materials. <i>Physical Review B</i> , 2016 , 93,	3.3	56
53	First-principles study of ground-state properties and high pressure behavior of ThO ₂ . <i>Journal of Nuclear Materials</i> , 2010 , 399, 181-188	3.3	54
52	Band-gap bowing and p-type doping of (Zn, Mg, Be)O wide-gap semiconductor alloys: a first-principles study. <i>European Physical Journal B</i> , 2008 , 66, 439-444	1.2	53

51	First-principles LDA+U and GGA+U study of neptunium dioxide. <i>Physical Review B</i> , 2010 , 81,	3.3	52
50	Broadband Emission in Hybrid Organic-Inorganic Halides of Group 12 Metals. <i>ACS Omega</i> , 2018 , 3, 18791-18802	3.5	47
49	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	3.6	44
48	First-Principles Study of Magnetic Properties of 3d Transition Metals Doped in ZnO Nanowires. <i>Nanoscale Research Letters</i> , 2009 , 4, 480-484	5	43
47	Zero-dimensional Cs ₄ EuX ₆ (X = Br, I) all-inorganic perovskite single crystals for gamma-ray spectroscopy. <i>Journal of Materials Chemistry C</i> , 2018 , 6, 6647-6655	7.1	40
46	Impact of metal ns ² lone pair on luminescence quantum efficiency in low-dimensional halide perovskites. <i>Physical Review Materials</i> , 2019 , 3,	3.2	40
45	Discrete Electronic Bands in Semiconductors and Insulators: Potential High-Light-Yield Scintillators. <i>Physical Review Applied</i> , 2015 , 3,	4.3	37
44	Electronic structures and mechanical properties of uranium monocarbide from first-principles LDA+U and GGA+U calculations. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2009 , 373, 3577-3581	2.3	35
43	Elasticity, band structure, and piezoelectricity of Be _x Zn _{1-x} O alloys. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2008 , 372, 2930-2933	2.3	34
42	Hybrid density functional theory study of band gap tuning in AlN and GaN through equibiaxial strains. <i>Applied Physics Letters</i> , 2012 , 100, 022104	3.4	32
41	Structural, electronic, and thermodynamic properties of UN: Systematic density functional calculations. <i>Journal of Nuclear Materials</i> , 2010 , 406, 218-222	3.3	29
40	Prospective high thermoelectric performance of the heavily p-doped half-Heusler compound CoVSn. <i>Physical Review B</i> , 2017 , 95,	3.3	26
39	Electronic and Magnetic Properties of Graphene/Fluorographene Superlattices. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 18278-18283	3.8	24
38	Magnetic behavior of Fe(Se,Te) systems: First-principles calculations. <i>Journal of Applied Physics</i> , 2011 , 110, 043917	2.5	23
37	Structural, electronic, mechanical, and thermodynamic properties of UN ₂ : Systematic density functional calculations. <i>Journal of Nuclear Materials</i> , 2011 , 410, 46-51	3.3	21
36	Magnetic coupling properties of Mn-doped ZnO nanowires: First-principles calculations. <i>Journal of Applied Physics</i> , 2008 , 103, 073903	2.5	21
35	Mechanical and chemical bonding properties of ground state BeH ₂ . <i>European Physical Journal B</i> , 2010 , 74, 303-308	1.2	20
34	Studies of tetragonal PbTiO ₃ subjected to uniaxial stress along the c-axis. <i>Journal of Physics Condensed Matter</i> , 2008 , 20, 175210	1.8	20

33	Structural, mechanical, thermodynamic, and electronic properties of thorium hydrides from first-principles. <i>Journal of Nuclear Materials</i> , 2010 , 401, 124-129	3.3	19
32	Scintillation Properties and Electronic Structures of the Intrinsic and Extrinsic Mixed Elpasolites Cs ₂ NaRBr ₃ I ₃ (R=La, Y). <i>Physical Review Applied</i> , 2016 , 5,	4.3	18
31	First-principles study of UC ₂ and U ₂ C ₃ . <i>Journal of Nuclear Materials</i> , 2010 , 396, 218-222	3.3	18
30	First-principles study of β -Pu ₂ O ₃ . <i>Journal of Nuclear Materials</i> , 2012 , 420, 159-163	3.3	17
29	Hybrid density functional theory studies of AlN and GaN under uniaxial strain. <i>Journal of Physics Condensed Matter</i> , 2013 , 25, 045801	1.8	17
28	Anomalous structural transformation, spontaneous polarization, piezoelectric response, and band structure of semiconductor aluminum nitride under hydrostatic pressure. <i>Journal of Applied Physics</i> , 2011 , 110, 103712	2.5	14
27	Crystal structure, electronic structure, temperature-dependent optical and scintillation properties of CsCe ₂ Br ₇ . <i>Journal of Materials Chemistry C</i> , 2015 , 3, 11366-11376	7.1	12
26	Phase transition and band-structure tuning in InN through uniaxial and biaxial strains. <i>Journal of Physics Condensed Matter</i> , 2014 , 26, 025501	1.8	10
25	Magnetic coupling properties of Mn-doped AlN nanowires: First-principles calculations. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2011 , 375, 1686-1689	2.3	10
24	Impurity-induced deep centers in Tl ₆ Si ₄ . <i>Journal of Applied Physics</i> , 2017 , 121, 145102	2.5	9
23	Lithium ion trapping mechanism of SiO in LiCoO based memristors. <i>Scientific Reports</i> , 2019 , 9, 5081	4.9	9
22	Magnetism in Na-filled Fe-based skutterudites. <i>Scientific Reports</i> , 2015 , 5, 10782	4.9	9
21	Stability and Repeatability of a Karst-like Hierarchical Porous Silicon Oxide-Based Memristor. <i>ACS Applied Materials & Interfaces</i> , 2019 , 11, 21734-21740	9.5	8
20	Doping Y ₂ O ₃ with Mn ⁴⁺ for energy-efficient lighting. <i>Journal of Materials Chemistry C</i> , 2018 , 6, 4171-4176	6.1	8
19	Ternary chalcogenides Cs ₂ Zn ₃ Se ₄ and Cs ₂ Zn ₃ Te ₄ : Potential p-type transparent conducting materials. <i>Physical Review B</i> , 2014 , 90,	3.3	8
18	Crystal structure, electronic structure, optical and scintillation properties of self-activated Cs ₄ YbI ₆ . <i>Journal of Luminescence</i> , 2018 , 201, 460-465	3.8	8
17	Native defects in Tl ₆ Si ₄ : Density functional calculations. <i>Journal of Applied Physics</i> , 2015 , 117, 175701	2.5	7
16	Strain-enhanced power conversion efficiency of a BP/SnSe van der Waals heterostructure. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 14787-14795	3.6	7

15	Barrier Reduction of Lithium Ion Tunneling through Graphene with Hybrid Defects: First-Principles Calculations. <i>Advanced Theory and Simulations</i> , 2018 , 1, 1700009	3.5	7
14	Li ₂ Se:Te as a neutron scintillator. <i>Journal of Alloys and Compounds</i> , 2015 , 647, 906-910	5.7	7
13	Electronic structure and magnetic coupling properties of Gd-doped AlN: first-principles calculations. <i>European Physical Journal B</i> , 2010 , 77, 345-349	1.2	7
12	Comparing the effects of uniaxial and biaxial strains on the structural stability and electronic structure in wurtzite ZnS. <i>Journal of Applied Physics</i> , 2013 , 114, 023514	2.5	6
11	Electron band structure of the high pressure cubic phase of AlH ₃ . <i>Journal of Physics: Conference Series</i> , 2012 , 377, 012093	0.3	6
10	p-type doping of GaInNAs quaternary alloys. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2008 , 373, 165-168	2.3	6
9	Tunable band offsets in the BP/PO van der Waals heterostructure: first-principles calculations. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 29931-29938	3.6	5
8	Ba ₂ TeO as an optoelectronic material: First-principles study. <i>Journal of Applied Physics</i> , 2015 , 117, 195705	5.5	3
7	Modulation of resistive switching in Pt/LiCoO ₂ /SiO ₂ /Si stacks. <i>Journal of Materials Science: Materials in Electronics</i> , 2019 , 30, 4753-4759	2.1	2
6	Electronic shell structures, self-trapped excitons, and defect-bound excitons in Li ₂ B ₁₂ H ₁₂ . <i>Journal of Materials Chemistry C</i> , 2019 , 7, 14342-14349	7.1	2
5	Competitive conductive mechanism of interstitial Ag and oxygen vacancies in Ag/Ta ₂ O ₅ /Pt stack. <i>Journal of Applied Physics</i> , 2019 , 126, 065104	2.5	1
4	Density functional studies of defects and defect-related luminescence in Mg ₃ N ₂ . <i>Physical Review Materials</i> , 2020 , 4,	3.2	1
3	Photophysical properties of zero-dimensional perovskites studied by PBE0 and GW+BSE methods. <i>Journal of Applied Physics</i> , 2021 , 130, 203106	2.5	1
2	Intrinsic and complex defect engineering of quasi-one-dimensional ribbons Sb ₂ S ₃ for photovoltaics performance. <i>Physical Review Materials</i> , 2021 , 5,	3.2	1
1	Anomalous optical and electronic properties of dense sodium. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2010 , 374, 4458-4464	2.3	