Hongliang Shi

List of Publications by Year
in descending order

68 papers	4,062 citations	172207 29 h-index	114278 63 g-index
68 all docs	68 docs citations	68 times ranked	6426 citing authors

#	Article	IF	Citations
1	Quasiparticle band structures and optical properties of strained monolayer MoS<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>and WS<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>. Physical Review B, 2013, 87, .	1.1	764
2	Mesoporous MnCeOx solid solutions for low temperature and selective oxidation of hydrocarbons. Nature Communications, 2015, 6, 8446.	5.8	241
3	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
4	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
5	Unraveling Thickness-Driven Dirac Fermion and Topological Insulator Behavior in Bi<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:m Bi<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
6	Electronic, transport, and optical properties of bulk and mono-layer PdSe2. Applied Physics Letters, 2015, 107, .	1.5	170
7	Unraveling luminescence mechanisms in zero-dimensional halide perovskites. Journal of Materials Chemistry C, 2018, 6, 6398-6405.	2.7	168
8	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
9	Fast Diffusion of Native Defects and Impurities in Perovskite Solar Cell Material CH₃NH₃PbI₃. Chemistry of Materials, 2016, 28, 4349-4357.	3.2	139
10	Strong ferromagnetism in hydrogenated monolayer MoS<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>tuned by strain. Physical Review B, 2013, 88, .	1.1	130
11	Nanoscale Transition Metal Dichalcogenides: Structures, Properties, and Applications. Critical Reviews in Solid State and Materials Sciences, 2014, 39, 319-367.	6.8	125
12	Shallow halogen vacancies in halide optoelectronic materials. Physical Review B, 2014, 90, .	1.1	119
13	Bismuth chalcohalides and oxyhalides as optoelectronic materials. Physical Review B, 2016, 93, .	1.1	82
14	Magnetic coupling properties of rare-earth metals (Gd, Nd) doped ZnO: First-principles calculations. Journal of Applied Physics, 2009, 106, .	1.1	76
15	Optical properties of UO2 and PuO2. Journal of Nuclear Materials, 2010, 400, 151-156.	1.3	72
16	Broadband Emission in Hybrid Organicâ€Inorganic Halides of Group 12 Metals. ACS Omega, 2018, 3, 18791-18802.	1.6	70
17	First-principles study of ground-state properties and high pressure behavior of ThO2. Journal of Nuclear Materials, 2010, 399, 181-188.	1.3	68
18	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

#	Article	IF	Citations
19	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.	0.6	63
20	First-principles<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>LDA</mml:mtext><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml:mrow></mml:math>a xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>GGA</mml:mtext><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml:mrow></mml:math> impact on metallic nickel. Physical Review B, 2010, 81, .	1.1	63
21	<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
22	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
23	Discrete Electronic Bands in Semiconductors and Insulators: Potential High-Light-Yield Scintillators. Physical Review Applied, 2015, 3, .	1.5	51
24	Electronic structures and mechanical properties of uranium monocarbide from first-principles and calculations. Physics Letters, Section A: General, Atomic and Solid State Physics, 2009, 373, 3577-3581.	0.9	46
25	First-Principles Study of Magnetic Properties of 3d Transition Metals Doped in ZnO Nanowires. Nanoscale Research Letters, 2009, 4, 480-484.	3.1	43
26	Hybrid density functional theory study of band gap tuning in AlN and GaN through equibiaxial strains. Applied Physics Letters, 2012, 100, .	1.5	41
27	Elasticity, band structure, and piezoelectricity of BexZn1â^'xO alloys. Physics Letters, Section A: General, Atomic and Solid State Physics, 2008, 372, 2930-2933.	0.9	37
28	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
29	Structural, electronic, and thermodynamic properties of UN: Systematic density functional calculations. Journal of Nuclear Materials, 2010, 406, 218-222.	1.3	34
30	Hybrid density functional theory studies of AlN and GaN under uniaxial strain. Journal of Physics Condensed Matter, 2013, 25, 045801.	0.7	28
31	Mechanical and chemical bonding properties of ground state BeH2. European Physical Journal B, 2010, 74, 303-308.	0.6	25
32	Electronic and Magnetic Properties of Graphene/Fluorographene Superlattices. Journal of Physical Chemistry C, 2012, 116, 18278-18283.	1.5	25
33	Structural, mechanical, thermodynamic, and electronic properties of thorium hydrides from first-principles. Journal of Nuclear Materials, 2010, 401, 124-129.	1.3	24
34	Structural, electronic, mechanical, and thermodynamic properties of UN2: Systematic density functional calculations. Journal of Nuclear Materials, 2011, 410, 46-51.	1.3	24
35	Stability and Repeatability of a Karst-like Hierarchical Porous Silicon Oxide-Based Memristor. ACS Applied Materials & Interfaces, 2019, 11, 21734-21740.	4.0	24
36	Studies of tetragonal PbTiO₃subjected to uniaxial stress along thec-axis. Journal of Physics Condensed Matter, 2008, 20, 175210.	0.7	23

#	Article	IF	Citations
37	First-principles study of UC2 and U2C3. Journal of Nuclear Materials, 2010, 396, 218-222.	1.3	23
38	Magnetic behavior of Fe(Se,Te) systems: First-principles calculations. Journal of Applied Physics, 2011, 110, .	1.1	23
39	Magnetic coupling properties of Mn-doped ZnO nanowires: First-principles calculations. Journal of Applied Physics, 2008, 103, 073903.	1.1	22
40	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:mi mathvariant="normal">I</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></m. Physical Review Applied, 2016, 5, .	1.5	22
41	Strain-enhanced power conversion efficiency of a BP/SnSe van der Waals heterostructure. Physical Chemistry Chemical Physics, 2020, 22, 14787-14795.	1.3	21
42	First-principles study of Î±-Pu2O3. Journal of Nuclear Materials, 2012, 420, 159-163.	1.3	19
43	Anomalous structural transformation, spontaneous polarization, piezoelectric response, and band structure of semiconductor aluminum nitride under hydrostatic pressure. Journal of Applied Physics, 2011, 110, 103712.	1.1	14
44	Crystal structure, electronic structure, temperature-dependent optical and scintillation properties of CsCe₂Br₇. Journal of Materials Chemistry C, 2015, 3, 11366-11376.	2.7	14
45	Lithium ion trapping mechanism of SiO2 in LiCoO2 based memristors. Scientific Reports, 2019, 9, 5081.	1.6	14
46	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.	0.9	12
47	Magnetism in Na-filled Fe-based skutterudites. Scientific Reports, 2015, 5, 10782.	1.6	12
48	Crystal structure, electronic structure, optical and scintillation properties of self-activated Cs4YbI6. Journal of Luminescence, 2018, 201, 460-465.	1.5	12
49	Barrier Reduction of Lithium Ion Tunneling through Graphene with Hybrid Defects: Firstâ€Principles Calculations. Advanced Theory and Simulations, 2018, 1, 1700009.	1.3	11
50	Phase transition and band-structure tuning in InN through uniaxial and biaxial strains. Journal of Physics Condensed Matter, 2014, 26, 025501.	0.7	10
51	Doping Y₂O₃ with Mn⁴⁺ for energy-efficient lighting. Journal of Materials Chemistry C, 2018, 6, 4171-4176.	2.7	10
52	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
53	Impurity-induced deep centers in Tl6SI4. Journal of Applied Physics, 2017, 121, 145102.	1.1	9
54	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:msub><mml:mi mathvariant="normal">S</mml:mi><mml:msub><mml:mi></mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> for photovoltaics performance. Physical Review Materials, 2021, 5, .	0.9	9

#	Article	IF	Citations
55	Electronic shell structures, self-trapped excitons, and defect-bound excitons in Li₂B₁₂H₁₂. Journal of Materials Chemistry C, 2019, 7, 14342-14349.	2.7	8
56	Electronic structure and magnetic coupling properties of Gd-doped AlN: first-principles calculations. European Physical Journal B, 2010, 77, 345-349.	0.6	7
57	Electron band structure of the high pressure cubic phase of AlH₃. Journal of Physics: Conference Series, 2012, 377, 012093.	0.3	7
58	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.	1.1	7
59	Li2Se:Te as a neutron scintillator. Journal of Alloys and Compounds, 2015, 647, 906-910.	2.8	7
60	Native defects in Tl6SI4: Density functional calculations. Journal of Applied Physics, 2015, 117, .	1.1	7
61	Tunable band offsets in the BP/P₄O₁₀ van der Waals heterostructure: first-principles calculations. Physical Chemistry Chemical Physics, 2018, 20, 29931-29938.	1.3	7
62	p-type doping of GaInNAs quaternary alloys. Physics Letters, Section A: General, Atomic and Solid State Physics, 2008, 373, 165-168.	0.9	6
63	Competitive conductive mechanism of interstitial Ag and oxygen vacancies in Ag/Ta2O5/Pt stack. Journal of Applied Physics, 2019, 126, .	1.1	4
64	Photophysical properties of zero-dimensional perovskites studied by PBE0 and GW+BSE methods. Journal of Applied Physics, 2021, 130, 203106.	1.1	4
65	Ba2TeO as an optoelectronic material: First-principles study. Journal of Applied Physics, 2015, 117, 195705.	1.1	3
66	Modulation of resistive switching in Pt/LiCoO2/SiO2/Si stacks. Journal of Materials Science: Materials in Electronics, 2019, 30, 4753-4759.	1.1	2
67	Density functional studies of defects and defect-related luminescence in Mg3N2. Physical Review Materials, 2020, 4, .	0.9	2
68	Anomalous optical and electronic properties of dense sodium. Physics Letters, Section A: General, Atomic and Solid State Physics, 2010, 374, 4458-4464.	0.9	0