Hezhu Shao

List of Publications by Year
in descending order

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100 papers	4,980 citations	76326 40 h-index	98798 67 g-index
101 all docs	101 docs citations	101 times ranked	5305 citing authors

#	Article	IF	Citations
1	The electronic, optical, and thermodynamic properties of borophene from first-principles calculations. Journal of Materials Chemistry C, 2016, 4, 3592-3598.	5.5	333
2	Thermal conductivity of monolayer MoS₂, MoSe₂, and WS₂: interplay of mass effect, interatomic bonding and anharmonicity. RSC Advances, 2016, 6, 5767-5773.	3.6	265
3	An excellent cyan-emitting orthosilicate phosphor for NUV-pumped white LED application. Journal of Materials Chemistry C, 2017, 5, 12365-12377.	5.5	203
4	Stability and strength of atomically thin borophene from first principles calculations. Materials Research Letters, 2017, 5, 399-407.	8.7	172
5	Phonon transport properties of two-dimensional group-IV materials from ab initio calculations. Physical Review B, 2016, 94, .	3.2	164
6	Low lattice thermal conductivity of stanene. Scientific Reports, 2016, 6, 20225.	3.3	161
7	Valence band engineering and thermoelectric performance optimization in SnTe by Mn-alloying via a zone-melting method. Journal of Materials Chemistry A, 2015, 3, 19974-19979.	10.3	141
8	The conflicting role of buckled structure in phonon transport of 2D group-IV and group-V materials. Nanoscale, 2017, 9, 7397-7407.	5.6	131
9	Firstâ€principle calculations of optical properties of monolayer arsenene and antimonene allotropes. Annalen Der Physik, 2017, 529, 1600152.	2.4	129
10	Enhanced thermoelectric performance in p-type polycrystalline SnSe benefiting from texture modulation. Journal of Materials Chemistry C, 2016, 4, 1201-1207.	5.5	125
11	Optimization of thermoelectric properties in n-type SnSe doped with BiCl3. Applied Physics Letters, 2016, 108, .	3.3	103
12	Manipulating Band Convergence and Resonant State in Thermoelectric Material SnTe by Mnâ€“In Codoping. ACS Energy Letters, 2017, 2, 1203-1207.	17.4	98
13	Water-mediated cation intercalation of open-framework indium hexacyanoferrate with high voltage and fast kinetics. Nature Communications, 2016, 7, 11982.	12.8	90
14	Methylsulfonylmethane-Based Deep Eutectic Solvent as a New Type of Green Electrolyte for a High-Energy-Density Aqueous Lithium-Ion Battery. ACS Energy Letters, 2019, 4, 1419-1426.	17.4	87
15	Band engineering and improved thermoelectric performance in M-doped SnTe (M = Mg, Mn, Cd, and Hg). Physical Chemistry Chemical Physics, 2016, 18, 7141-7147.	2.8	86
16	First-principles study on the electronic, optical, and transport properties of monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î±</mml:mi></mml:math> - and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î²</mml:mi></mml:math> -GeSe. Physical Review B, 2017, 96, .	3.2	81
17	Chemical intuition for high thermoelectric performance in monolayer black phosphorus, Î±-arsenene and aW-antimonene. Journal of Materials Chemistry A, 2018, 6, 2018-2033.	10.3	80
18	High thermoelectric performance in two-dimensional graphyne sheets predicted by first-principles calculations. Physical Chemistry Chemical Physics, 2015, 17, 22872-22881.	2.8	77

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19	Designing band engineering for thermoelectrics starting from the periodic table of elements. Materials Today Physics, 2018, 7, 35-44.	6.0	75
20	Ion-selective copper hexacyanoferrate with an open-framework structure enables high-voltage aqueous mixed-ion batteries. Journal of Materials Chemistry A, 2017, 5, 16740-16747.	10.3	74
21	Enhanced thermopower in rock-salt SnTeâ€“CdTe from band convergence. RSC Advances, 2016, 6, 32189-32192.	3.6	72
22	Ultra-stable sodium metal-iodine batteries enabled by an in-situ solid electrolyte interphase. Nano Energy, 2019, 57, 692-702.	16.0	72
23	First-Principles Prediction of Ultralow Lattice Thermal Conductivity of Dumbbell Silicene: A Comparison with Low-Buckled Silicene. ACS Applied Materials & Interfaces, 2016, 8, 20977-20985.	8.0	66
24	Towards intrinsic phonon transport in singleâ€layer MoS₂. Annalen Der Physik, 2016, 528, 504-511.	2.4	65
25	1D SbSeI, SbSI, and SbSBr With High Stability and Novel Properties for Microelectronic, Optoelectronic, and Thermoelectric Applications. Advanced Theory and Simulations, 2018, 1, 1700005.	2.8	65
26	YAGG:Ce transparent ceramics with high luminous efficiency for solid-state lighting application. Journal of Advanced Ceramics, 2019, 8, 389-398.	17.4	56
27	Numerical solutions of the time-dependent SchrÃ¶dinger equation: Reduction of the error due to space discretization. Physical Review E, 2009, 79, 056705.	2.1	53
28	Unlocking Fewâ€Layered Ternary Chalcogenides for Highâ€Performance Potassiumâ€Ion Storage. Advanced Energy Materials, 2019, 9, 1901560.	19.5	53
29	A first-principles study on the phonon transport in layered BiCuOSe. Scientific Reports, 2016, 6, 21035.	3.3	52
30	Arbitrarily precise numerical solutions of the one-dimensional SchrÃ¶dinger equation. Computer Physics Communications, 2009, 180, 1-7.	7.5	50
31	A new kind of discretization scheme for solving a two-dimensional time-independent SchrÃ¶dinger equation. Computer Physics Communications, 2009, 180, 842-849.	7.5	50
32	Texturing degree boosts thermoelectric performance of silver-doped polycrystalline SnSe. NPG Asia Materials, 2017, 9, e426-e426.	7.9	49
33	A nitrogen-hyperdoped silicon material formed by femtosecond laser irradiation. Applied Physics Letters, 2014, 104, .	3.3	47
34	High thermoelectric performance of Weyl semimetal TaAs. Nano Energy, 2016, 30, 225-234.	16.0	47
35	The role of Andersonâ€™s rule in determining electronic, optical and transport properties of transition metal dichalcogenide heterostructures. Physical Chemistry Chemical Physics, 2018, 20, 30351-30364.	2.8	47
36	Improving Thermoelectric Performance of Î±â€MgAgSb by Theoretical Band Engineering Design. Advanced Energy Materials, 2017, 7, 1700076.	19.5	46

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37	Optimizing the thermoelectric performance of Inâ€“Cd codoped SnTe by introducing Sn vacancies. Journal of Materials Chemistry C, 2017, 5, 7504-7509.	5.5	46
38	Inâ€Plane Anisotropic Thermal Conductivity of Fewâ€Layered Transition Metal Dichalcogenide Tdâ€WTe₂. Advanced Materials, 2019, 31, e1804979.	21.0	45
39	Highly-accurate ground state energies of the He atom and the He-like ions by Hartree SCF calculation with Obrechkoff method. Computer Physics Communications, 2008, 179, 486-491.	7.5	44
40	Thermoelectric properties of In-Hg co-doping in SnTe: Energy band engineering. Journal of Materiomics, 2018, 4, 62-67.	5.7	44
41	Sub-picosecond photo-induced displacive phase transition in two-dimensional MoTe2. Npj 2D Materials and Applications, 2020, 4, .	7.9	43
42	Charge Transport in Thermoelectric SnSe Single Crystals. ACS Energy Letters, 2018, 3, 689-694.	17.4	41
43	Enhanced thermoelectric performance in n-type polycrystalline SnSe by PbBr₂ doping. RSC Advances, 2017, 7, 17906-17912.	3.6	40
44	Room Temperature Bound Excitons and Strain-Tunable Carrier Mobilities in Janus Monolayer Transition-Metal Dichalcogenides. Journal of Physical Chemistry Letters, 2020, 11, 3116-3128.	4.6	38
45	Physical mechanisms for the unique optical properties of chalcogen-hyperdoped silicon. Europhysics Letters, 2012, 99, 46005.	2.0	37
46	Element-selective resonant state in M-doped SnTe (M = Ga, In, and Tl). Physical Chemistry Chemical Physics, 2016, 18, 20635-20639.	2.8	37
47	Insights into High Conductivity of the Two-Dimensional Iodine-Oxidized sp²-c-COF. ACS Applied Materials & Interfaces, 2018, 10, 43595-43602.	8.0	37
48	Nontrivial thermoelectric behavior in cubic SnSe driven by spin-orbit coupling. Nano Energy, 2018, 51, 649-655.	16.0	37
49	Thermoelectric (Bi,Sb)2Te3â€“Ge0.5Mn0.5Te composites with excellent mechanical properties. Journal of Materials Chemistry A, 2019, 7, 9241-9246.	10.3	37
50	Beyond Perturbation: Role of Vacancy-Induced Localized Phonon States in Thermal Transport of Monolayer MoS₂. Journal of Physical Chemistry C, 2016, 120, 29324-29331.	3.1	36
51	Ultralow Lattice Thermal Conductivity in SnTe by Manipulating the Electronâ€“Phonon Coupling. Journal of Physical Chemistry C, 2019, 123, 15996-16002.	3.1	36
52	Band engineering and crystal field screening in thermoelectric Mg₃Sb₂. Journal of Materials Chemistry A, 2019, 7, 8922-8928.	10.3	36
53	Discovery of Leadâ€Free Perovskites for Highâ€Performance Solar Cells via Machine Learning: Ultrabroadband Absorption, Low Radiative Combination, and Enhanced Thermal Conductivities. Advanced Science, 2022, 9, e2103648.	11.2	35
54	Electronic Band Structure and Sub-band-gap Absorption of Nitrogen Hyperdoped Silicon. Scientific Reports, 2015, 5, 10513.	3.3	31

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55	Synthesis of SnTe/AgSbSe 2 nanocomposite as a promising lead-free thermoelectric material. Journal of Materiomics, 2016, 2, 165-171.	5.7	31
56	Room-Temperature Bound Exciton with Long Lifetime in Monolayer GaN. ACS Photonics, 2018, 5, 4081-4088.	6.6	30
57	Synergistic Optimization of Thermoelectric Performance in P-Type Bi0.48Sb1.52Te3/Graphene Composite. Energies, 2016, 9, 236.	3.1	29
58	Study on Thermoelectric Properties of Polycrystalline SnSe by Ge Doping. Journal of Electronic Materials, 2017, 46, 3182-3186.	2.2	29
59	High thermoelectric efficiency in monolayer PbI₂ from 300 K to 900 K. Inorganic Chemistry Frontiers, 2019, 6, 920-928.	6.0	29
60	Single crystal growth of Sn 0.97 Ag 0.03 Se by a novel horizontal Bridgman method and its thermoelectric properties. Journal of Crystal Growth, 2017, 460, 112-116.	1.5	28
61	Anisotropic ultrahigh hole mobility in two-dimensional penta-SiC₂ by strain-engineering: electronic structure and chemical bonding analysis. RSC Advances, 2017, 7, 45705-45713.	3.6	28
62	Thermoelectric properties of textured polycrystalline Na_{0.03}Sn_{0.97}Se enhanced by hot deformation. Journal of Materials Chemistry A, 2018, 6, 23730-23735.	10.3	27
63	Remarkable intrinsic ZT in the 2D PtX2(XÂ=ÂO, S, Se, Te) monolayers at room temperature. Applied Surface Science, 2020, 532, 147387.	6.1	27
64	Strong Mid-Infrared Absorption and High Crystallinity of Microstructured Silicon Formed by Femtosecond Laser Irradiation in NF₃Atmosphere. Applied Physics Express, 2013, 6, 081301.	2.4	26
65	Tuning Thermal Transport in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mrow><mml:mrow><mml:mi mathvariant="normal">C</mml:mi></mml:mrow></mml:mrow><mml:mn>3</mml:mn></mml:msub><mml:mrow><mml:mi mathvariant="normal">N</mml:mi></mml:mrow></mml:math> Monolayers by Adding and Removing Carbon Atoms. Physical Review Applied, 2018, 10, .	3.8	25
66	Thermoelectric performance of 2D materials: the band-convergence strategy and strong intervalley scatterings. Materials Horizons, 2021, 8, 1253-1263.	12.2	25
67	Theoretical understanding on band engineering of Mn-doped lead chalcogenides PbX (X = Te, Se, S). Journal of Physics Condensed Matter, 2015, 27, 095501.	1.8	22
68	First-principles study on the elastic properties of Cu ₂ GeSe ₃. Europhysics Letters, 2016, 113, 26001.	2.0	22
69	Growth and characterization of large size undoped p -type SnSe single crystal by Horizontal Bridgman method. Journal of Alloys and Compounds, 2017, 712, 857-862.	5.5	21
70	Acoustic phonon softening and reduced thermal conductivity in Mg2Si1â^'xSnx solid solutions. Applied Physics Letters, 2017, 110, .	3.3	21
71	First-principles study on the lattice dynamics and thermodynamic properties of Cu ₂ GeSe ₃. Europhysics Letters, 2015, 109, 47004.	2.0	20
72	Optimized orientation and enhanced thermoelectric performance in Sn_{0.97}Na_{0.03}Se with Te addition. Journal of Materials Chemistry C, 2019, 7, 2653-2658.	5.5	19

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73	Strong electronâ€“phonon coupling influences carrier transport and thermoelectric performances in group-IV/V elemental monolayers. Npj Computational Materials, 2021, 7, .	8.7	19
74	Hybrid Functional Studies on Impurity-Concentration-Controlled Band Engineering of Chalcogen-Hyperdoped Silicon. Applied Physics Express, 2013, 6, 085801.	2.4	18
75	Microstructure engineering beyond SnSe1-xSx solid solution for high thermoelectric performance. Journal of Materiomics, 2018, 4, 321-328.	5.7	18
76	Structure and thermoelectric properties of the n-type clathrate Ba8Cu5.1Ge40.2Sn0.7. Journal of Materials Chemistry A, 2015, 3, 19100-19106.	10.3	17
77	Enhanced thermoelectric performance in p-type polycrystalline SnSe by Cu doping. Journal of Materials Science: Materials in Electronics, 2018, 29, 18727-18732.	2.2	17
78	Ultrafine Gd 2 O 2 S:Pr powders prepared via urea precipitation method using SO 2 /SO 4 2â^' as sulfuration agentâ€"A comparative study. Powder Technology, 2017, 305, 382-388.	4.2	15
79	Anomalous lattice thermal conductivity in layered MNCl (M = Zr, Hf) materials driven by lanthanide contraction. Journal of Materials Chemistry A, 2020, 8, 3128-3134.	10.3	14
80	Theoretical investigations of Janus WSeTe monolayer and related van der Waals heterostructures with promising thermoelectric performance. Applied Surface Science, 2022, 593, 153402.	6.1	14
81	Enhanced power factor in the promising thermoelectric material SnPb_xTe prepared via zone-melting. RSC Advances, 2015, 5, 59379-59383.	3.6	13
82	Pushing Optical Switch into Deep Mid-Infrared Region: Band Theory, Characterization, and Performance of Topological Semimetal Antimonene. ACS Nano, 2021, 15, 7430-7438.	14.6	13
83	Possible atomic structures responsible for the sub-bandgap absorption of chalcogen-hyperdoped silicon. Applied Physics Letters, 2015, 107, 112106.	3.3	11
84	Texture Development and Grain Alignment of Hotâ€Pressed Tetradymite Bi_{0.48}Sb_{1.52}Te₃ via Powder Molding. Energy Technology, 2019, 7, 1900814.	3.8	11
85	Two-dimensional semiconducting gold. Physical Review B, 2017, 95, .	3.2	10
86	Stabilization of Thermoelectric Properties of the Cu/Bi0.48Sb1.52Te3 Composite for Advantageous Power Generation. Journal of Electronic Materials, 2017, 46, 2746-2751.	2.2	9
87	Investigation on structure and thermoelectric properties in p-type Bi0.48Sb1.52Te3 via PbTe incorporating. Journal of Materials Science: Materials in Electronics, 2018, 29, 7701-7706.	2.2	9
88	Zintl Phase Compounds Mg3Sb2â^'xBix (x = 0, 1, and 2) Monolayers: Electronic, Phonon and Thermoelectric Properties From ab Initio Calculations. Frontiers in Mechanical Engineering, 2022, 8, .	1.8	7
89	A first-principles study on the intrinsic phonon transport of Cu 2 GeSe 3. Europhysics Letters, 2016, 115, 26002.	2.0	6
90	First-Principles Study of Manipulating the Phonon Transport of Molybdenum Disulfide by Sodium Intercalating. Journal of Physical Chemistry C, 2018, 122, 2632-2640.	3.1	6

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91	High intrinsic ZT in InP₃ monolayer at room temperature. Journal of Physics Condensed Matter, 2019, 31, 365501.	1.8	6
92	Atomic scale study of stress-induced misaligned subsurface layers in KDP crystals. Scientific Reports, 2019, 9, 10399.	3.3	5
93	Towards high-temperature electron-hole condensate phases in monolayer tetrels metal halides: Ultra-long excitonic lifetimes, phase diagram and exciton dynamics. Materials Today Physics, 2022, 22, 100604.	6.0	5
94	Atomic dynamics of stress-induced lattice misalignment structures in a KDP subsurface. RSC Advances, 2020, 10, 23944-23952.	3.6	4
95	Renormalized thermoelectric figure of merit in a band-convergent Sb₂Te₂Se monolayer: full electronâ€“phonon interactions and selection rules. Journal of Materials Chemistry A, 2021, 9, 16108-16118.	10.3	4
96	Thermoelectric performance in a Si allotrope with ultralow thermal conductivity: a first-principles study combining phonon-limited electronic transport calculations. Materials Today Physics, 2022, 27, 100756.	6.0	3
97	Site-selective substitutional doping with atomic precision on stepped Al (111) surface by single-atom manipulation. Nanoscale Research Letters, 2014, 9, 235.	5.7	2
98	Low-energy structures of clusters supported on metal fcc(110) surfaces. Nanoscale Research Letters, 2011, 6, 633.	5.7	0
99	Reliable Lateral Atom Manipulation by Thermal Activation on Metal fcc(001) Surfaces. Journal of the Physical Society of Japan, 2013, 82, 104602.	1.6	0
100	Three-dimensional hybridized carbon networks for high performance thermoelectric applications. RSC Advances, 2014, 4, 42234-42239.	3.6	0