

Shiqiang Hao

List of Publications by Year in descending order

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101
papers

8,764
citations

66315

42
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42364

92
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102
all docs

102
docs citations

102
times ranked

7004
citing authors

#	ARTICLE	IF	CITATIONS
1	Thermoelectric Performance of the 2D Bi ₂ Si ₂ Te ₆ Semiconductor. <i>Journal of the American Chemical Society</i> , 2022, 144, 1445-1454.	6.6	37
2	Extraordinary role of Zn in enhancing thermoelectric performance of Ga-doped n-type PbTe. <i>Energy and Environmental Science</i> , 2022, 15, 368-375.	15.6	107
3	Weak-Bonding Elements Lead to High Thermoelectric Performance in BaSnS ₃ and SrSnS ₃ : A First-Principles Study. <i>Chemistry of Materials</i> , 2022, 34, 1289-1301.	3.2	19
4	Synergistic defect- and interfacial-engineering of a Bi ₂ S ₃ -based nanoplate network for high-performance photoelectrochemical solar water splitting. <i>Journal of Materials Chemistry A</i> , 2022, 10, 7830-7840.	5.2	13
5	Valence Disproportionation of GeS in the PbS Matrix Forms Pb ₅ Ge ₅ S ₁₂ Inclusions with Conduction Band Alignment Leading to High n-Type Thermoelectric Performance. <i>Journal of the American Chemical Society</i> , 2022, 144, 7402-7413.	6.6	24
6	High Thermoelectric Performance in Chalcopyrite Cu ₂ Ag ₂ GaTe ₂ ZnTe: Nontrivial Band Structure and Dynamic Doping Effect. <i>Journal of the American Chemical Society</i> , 2022, 144, 9113-9125.	6.6	29
7	Antimony doping to enhance luminescence of tin(IV)-based hybrid metal halides. <i>Inorganic Chemistry Frontiers</i> , 2022, 9, 3865-3873.	3.0	9
8	Probing the Optical Response and Local Dielectric Function of an Unconventional Si@MoS ₂ Core-Shell Architecture. <i>Nano Letters</i> , 2022, 22, 4848-4853.	4.5	2
9	In ₄ Pb _{5.5} Sb ₅ S ₁₉ : A Stable Quaternary Chalcogenide with Low Thermal Conductivity. <i>Inorganic Chemistry</i> , 2021, 60, 325-333.	1.9	5
10	Strong Valence Band Convergence to Enhance Thermoelectric Performance in PbSe with Two Chemically Independent Controls. <i>Angewandte Chemie</i> , 2021, 133, 272-277.	1.6	7
11	Strong Valence Band Convergence to Enhance Thermoelectric Performance in PbSe with Two Chemically Independent Controls. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 268-273.	7.2	28
12	Raspberry-like mesoporous Co-doped TiO ₂ nanospheres for a high-performance formaldehyde gas sensor. <i>Journal of Materials Chemistry A</i> , 2021, 9, 6529-6537.	5.2	33
13	Sn ₄ B ₁₂ Se ₁₂ [Q _x], Q = Se, Te, a B ₁₂ Cluster Tunnel Framework Hosting Neutral Chalcogen Chains. <i>Chemistry of Materials</i> , 2021, 33, 1723-1730.	3.2	6
14	Dissociation of GaSb in n-Type PbTe: off-Centered Gallium Atom and Weak Electron-Phonon Coupling Provide High Thermoelectric Performance. <i>Chemistry of Materials</i> , 2021, 33, 1842-1851.	3.2	23
15	Lithium Thiostannate Spinels: Air-Stable Cubic Semiconductors. <i>Chemistry of Materials</i> , 2021, 33, 2080-2089.	3.2	6
16	Implications of doping on microstructure, processing, and thermoelectric performance: The case of PbSe. <i>Journal of Materials Research</i> , 2021, 36, 1272-1284.	1.2	8
17	Ultralow Thermal Conductivity in Diamondoid Structures and High Thermoelectric Performance in (Cu ₂ Ag)(In ₂ Ga ₂)Te ₈ . <i>Journal of the American Chemical Society</i> , 2021, 143, 5978-5989.	3.2	49
18	Vast Structural and Polymorphic Varieties of Semiconductors AMM ₂ Q ₄ (A = K, Rb, Cs, Tl; M = Ga, In; M ₂ =) Tj ETQq0 0 0 rgBT /Over	3.2	6

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19	Broad Photoluminescence and Second-Harmonic Generation in the Noncentrosymmetric Organic-Inorganic Hybrid Halide $(\text{C}_6\text{H}_5\text{CH}_2)_4\text{N}_3\text{MX}_7\text{A}_2$ ($\text{M} = \text{Bi, In, X} = \text{Br or I}$). <i>Chemistry of Materials</i> , 2021, 33, 8106-8111.	8.2	36
20	Structure Tuning, Strong Second Harmonic Generation Response, and High Optical Stability of the Polar Semiconductors $\text{Na}_2\text{KAs}_2\text{Q}_2$. <i>Journal of the American Chemical Society</i> , 2021, 143, 18204-18215.	6.6	24
21	Broadband light emitting zero-dimensional antimony and bismuth-based hybrid halides with diverse structures. <i>Journal of Materials Chemistry C</i> , 2021, 9, 15942-15948.	2.7	18
22	Decreasing Structural Dimensionality of Double Perovskites for Phase Stabilization toward Efficient X-ray Detection. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 61447-61453.	4.0	11
23	Optical phonon dominated heat transport: A first-principles thermal conductivity study of BaSnS_2 . <i>Physical Review B</i> , 2021, 104, .	11.7	12
24	Discordant nature of Cd in PbSe: off-centering and core-shell nanoscale CdSe precipitates lead to high thermoelectric performance. <i>Energy and Environmental Science</i> , 2020, 13, 200-211.	15.6	57
25	Discordant nature of Cd in GeTe enhances phonon scattering and improves band convergence for high thermoelectric performance. <i>Journal of Materials Chemistry A</i> , 2020, 8, 1193-1204.	5.2	83
26	High-Performance Thermoelectrics from Cellular Nanostructured $\text{Sb}_2\text{Si}_2\text{Te}_6$. <i>Joule</i> , 2020, 4, 159-175.	11.7	103
27	Superior Oxygen Reduction Reaction on Phosphorus-Doped Carbon Dot/Graphene Aerogel for All-Solid-State Flexible Air Batteries. <i>Advanced Energy Materials</i> , 2020, 10, 1902736.	10.2	93
28	High Thermoelectric Performance in the New Cubic Semiconductor $\text{Ag}_3\text{SnSbSe}_3$ by High-Entropy Engineering. <i>Journal of the American Chemical Society</i> , 2020, 142, 15187-15198.	6.6	108
29	Layered and Cubic Semiconductors GaM_2Q_4 ($\text{A} = \text{Ga, In, Tl}$; $\text{M} = \text{Sb, Bi}$; $\text{Q} = \text{S, Se, Te}$). <i>Journal of Materials Chemistry A</i> , 2020, 8, 1193-1204.	6.6	21
30	Ultralow thermal conductivity in diamondoid lattices: high thermoelectric performance in chalcopyrite $\text{Cu}_{0.8}\text{Ag}_{0.2}\text{In}_2\text{Te}_2$. <i>Energy and Environmental Science</i> , 2020, 13, 3693-3705.	15.6	52
31	Identifying the Origins of High Thermoelectric Performance in Group IIIA Element Doped PbS. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 14203-14212.	4.0	12
32	Crystal structure and luminescence properties of lead-free metal halides $(\text{C}_6\text{H}_5\text{CH}_2)_3\text{MBr}_6$ ($\text{M} = \text{Bi}$). <i>Journal of Materials Chemistry C</i> , 2020, 8, 1193-1204.	11.7	103
33	Ultralow Thermal Conductivity and Thermoelectric Properties of $\text{Rb}_2\text{Bi}_8\text{Se}_{13}$. <i>Chemistry of Materials</i> , 2020, 32, 3561-3569.	3.2	23
34	Direct Visualization of Electric-Field-Induced Structural Dynamics in Monolayer Transition Metal Dichalcogenides. <i>ACS Nano</i> , 2020, 14, 1569-1576.	7.3	23
35	All-Inorganic Halide Perovskites as Potential Thermoelectric Materials: Dynamic Cation off-Centering Induces Ultralow Thermal Conductivity. <i>Journal of the American Chemical Society</i> , 2020, 142, 9553-9563.	6.6	155
36	Topology of transition metal dichalcogenides: the case of the core-shell architecture. <i>Nanoscale</i> , 2020, 12, 23897-23919.	2.8	14

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37	Quasilinear dispersion in electronic band structure and high Seebeck coefficient in CuFeS_2 -based thermoelectric materials. <i>Physical Review Materials</i> , 2020, 4, .	0.9	7
38	Ion Beam Induced Artifacts in Lead Based Chalcogenides. <i>Microscopy and Microanalysis</i> , 2019, 25, 2262-2263.	0.2	1
39	Ultralow Thermal Conductivity and High-Temperature Thermoelectric Performance in n-Type $\text{K}_{2.5}\text{Bi}_{8.5}\text{Se}_{14}$. <i>Chemistry of Materials</i> , 2019, 31, 5943-5952.	3.2	25
40	Large Thermal Conductivity Drops in the Diamondoid Lattice of CuFeS_2 by Discordant Atom Doping. <i>Journal of the American Chemical Society</i> , 2019, 141, 18900-18909.	6.6	66
41	Lead-Free Broadband Orange-Emitting Zero-Dimensional Hybrid $(\text{PMA})_3\text{InBr}_6$ with Direct Band Gap. <i>Inorganic Chemistry</i> , 2019, 58, 15602-15609.	1.9	81
42	High Figure of Merit in Gallium-Doped Nanostructured n-Type PbTe_xGeTe with Midgap States. <i>Journal of the American Chemical Society</i> , 2019, 141, 16169-16177.	6.6	76
43	MoS_2 -capped Cu_xS nanocrystals: a new heterostructured geometry of transition metal dichalcogenides for broadband optoelectronics. <i>Materials Horizons</i> , 2019, 6, 587-594.	6.4	18
44	Origin of Intrinsically Low Thermal Conductivity in Talnakhite $\text{Cu}_{17.6}\text{Fe}_{17.6}\text{S}_{32}$ Thermoelectric Material: Correlations between Lattice Dynamics and Thermal Transport. <i>Journal of the American Chemical Society</i> , 2019, 141, 10905-10914.	6.6	50
45	Ion Beam Induced Artifacts in Lead-Based Chalcogenides. <i>Microscopy and Microanalysis</i> , 2019, 25, 831-839.	0.2	6
46	Computational strategies for design and discovery of nanostructured thermoelectrics. <i>Npj Computational Materials</i> , 2019, 5, .	3.5	39
47	Design Strategy for High-Performance Thermoelectric Materials: The Prediction of Electron-Doped KZrCuSe_3 . <i>Chemistry of Materials</i> , 2019, 31, 3018-3024.	3.2	23
48	Enhancement of Thermoelectric Performance for n-Type PbS through Synergy of Gap State and Fermi Level Pinning. <i>Journal of the American Chemical Society</i> , 2019, 141, 6403-6412.	6.6	67
49	Six Quaternary Chalcogenides of the Pavonite Homologous Series with Ultralow Lattice Thermal Conductivity. <i>Chemistry of Materials</i> , 2019, 31, 3430-3439.	3.2	28
50	Enhanced Density-of-States Effective Mass and Strained Endotaxial Nanostructures in Sb-Doped $\text{Pb}_{0.97}\text{Cd}_{0.03}\text{Te}$ Thermoelectric Alloys. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 9197-9204.	4.0	66
51	Probing Strain-Induced Band Gap Modulation in 2D Hybrid Organic-Inorganic Perovskites. <i>ACS Energy Letters</i> , 2019, 4, 796-802.	8.8	47
52	All-Scale Hierarchically Structured p-Type PbSe Alloys with High Thermoelectric Performance Enabled by Improved Band Degeneracy. <i>Journal of the American Chemical Society</i> , 2019, 141, 4480-4486.	6.6	87
53	Thermoelectric Material $\text{SnPb}_2\text{Bi}_2\text{S}_6$: The 4,4L Member of Lillianite Homologous Series with Low Lattice Thermal Conductivity. <i>Inorganic Chemistry</i> , 2019, 58, 1339-1348.	1.9	10
54	High Thermoelectric Performance in the Wide Bandgap $\text{AgGa}_{1-x}\text{Te}_2$ Compounds: Directional Negative Thermal Expansion and Intrinsically Low Thermal Conductivity. <i>Advanced Functional Materials</i> , 2019, 29, 1806534.	7.8	65

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55	Computational prediction of nanostructured alloys with enhanced thermoelectric properties. <i>Physical Review Materials</i> , 2019, 3, .	0.9	3
56	Dimensionally driven crossover from semimetal to direct semiconductor in layered SbAs. <i>Physical Review Materials</i> , 2019, 3, .	0.9	1
57	Intrinsic Transport in 2D Heterostructures Mediated through h-BN Tunneling Contacts. <i>Nano Letters</i> , 2018, 18, 2990-2998.	4.5	39
58	First-Principles Study of Lithium Cobalt Spinel Oxides: Correlating Structure and Electrochemistry. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 13479-13490.	4.0	31
59	Optically Active 1D MoS ₂ Nanobelts. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 6799-6804.	4.0	23
60	High Thermoelectric Performance in SnTe/AgSbTe ₂ Alloys from Lattice Softening, Giant Phonon Vacancy Scattering, and Valence Band Convergence. <i>ACS Energy Letters</i> , 2018, 3, 705-712.	8.8	151
61	Large-scale Fabrication of MoS ₂ Ribbons and Their Light-induced Electronic/Thermal Properties: Dichotomies in the Structural and Defect Engineering. <i>Advanced Functional Materials</i> , 2018, 28, 1704863.	7.8	25
62	Quaternary Pavonites A _{1-x} Sn _{2x} Bi _{5-x} S ₁₀ (A ⁺ = Li ⁺ , Na ⁺): Site Occupancy Disorder Defines Electronic Structure. <i>Inorganic Chemistry</i> , 2018, 57, 2260-2268.	1.9	12
63	Grain Boundaries Softening Thermoelectric Oxide BiCuSeO. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 6772-6777.	4.0	10
64	Rhombohedral to Cubic Conversion of GeTe via MnTe Alloying Leads to Ultralow Thermal Conductivity, Electronic Band Convergence, and High Thermoelectric Performance. <i>Journal of the American Chemical Society</i> , 2018, 140, 2673-2686.	6.6	307
65	High thermoelectric performance in Bi _{0.46} Sb _{1.54} Te ₃ nanostructured with ZnTe. <i>Energy and Environmental Science</i> , 2018, 11, 1520-1535.	15.6	239
66	n-type SnSe ₂ Oriented Nanoplate-Based Pellets for High Thermoelectric Performance. <i>Advanced Energy Materials</i> , 2018, 8, 1702167.	10.2	103
67	First-principles calculations and experimental studies of XYZ ₂ thermoelectric compounds: detailed analysis of van der Waals interactions. <i>Journal of Materials Chemistry A</i> , 2018, 6, 19502-19519.	5.2	20
68	Chemical Insights into PbSe/HgSe: High Power Factor and Improved Thermoelectric Performance by Alloying with Discordant Atoms. <i>Journal of the American Chemical Society</i> , 2018, 140, 18115-18123.	6.6	80
69	Dual Alloying Strategy to Achieve a High Thermoelectric Figure of Merit and Lattice Hardening in p-Type Nanostructured PbTe. <i>ACS Energy Letters</i> , 2018, 3, 2593-2601.	8.8	37
70	Weak Electron Phonon Coupling and Deep Level Impurity for High Thermoelectric Performance Pb _{1-x} Ga _x Te. <i>Advanced Energy Materials</i> , 2018, 8, 1800659.	10.2	111
71	Absence of Nanostructuring in NaPb _m SbTe _{m+2} : Solid Solutions with High Thermoelectric Performance in the Intermediate Temperature Regime. <i>Journal of the American Chemical Society</i> , 2018, 140, 7021-7031.	6.6	27
72	Quaternary Chalcogenide Semiconductors with 2D Structures: Rb ₂ ZnBi ₂ Se ₅ and Cs ₆ Cd ₂ Bi ₈ Te ₁₇ . <i>Inorganic Chemistry</i> , 2018, 57, 9403-9411.	1.9	10

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73	Ni and Se co-doping increases the power factor and thermoelectric performance of CoSbS. <i>Journal of Materials Chemistry A</i> , 2018, 6, 15123-15131.	5.2	20
74	Soft phonon modes from off-center Ge atoms lead to ultralow thermal conductivity and superior thermoelectric performance in n-type PbSe ϵ GeSe. <i>Energy and Environmental Science</i> , 2018, 11, 3220-3230.	15.6	115
75	The New Semiconductor Cs ₄ Cu ₃ Bi ₉ S ₁₇ . <i>Chemistry of Materials</i> , 2017, 29, 1744-1751.	3.2	13
76	Systematic Study of Oxygen Vacancy Tunable Transport Properties of Few-Layer MoO ₃ Enabled by Vapor-Based Synthesis. <i>Advanced Functional Materials</i> , 2017, 27, 1605380.	7.8	91
77	High Thermoelectric Performance in Electron-Doped AgBi ₃ S ₅ with Ultralow Thermal Conductivity. <i>Journal of the American Chemical Society</i> , 2017, 139, 6467-6473.	6.6	160
78	Bi ₂ PdO ₄ : A Promising Thermoelectric Oxide with High Power Factor and Low Lattice Thermal Conductivity. <i>Chemistry of Materials</i> , 2017, 29, 2529-2534.	3.2	42
79	In-situ Electron Diffraction Studies of Sodium Electrochemistry in MoS ₂ . <i>Microscopy and Microanalysis</i> , 2017, 23, 2050-2051.	0.2	0
80	Homologous Series of 2D Chalcogenides CsAgBi ₂ Q (Q = S, Se) with Ion-Exchange Properties. <i>Journal of the American Chemical Society</i> , 2017, 139, 12601-12609.	6.6	22
81	Pressure induced thermoelectric enhancement in SnSe crystals. <i>Journal of Materials Chemistry A</i> , 2016, 4, 12073-12079.	5.2	81
82	Microstructure Evolution in Nanostructured High-Performance Thermoelectrics: The case of p-type Pb _{1-x} Na _x Te-SrTe. <i>Microscopy and Microanalysis</i> , 2016, 22, 1268-1269.	0.2	0
83	High-throughput computational design of cathode coatings for Li-ion batteries. <i>Nature Communications</i> , 2016, 7, 13779.	5.8	145
84	Research Update: Prediction of high figure of merit plateau in SnS and solid solution of (Pb,Sn)S. <i>APL Materials</i> , 2016, 4, .	2.2	29
85	Computational Prediction of High Thermoelectric Performance in Hole Doped Layered GeSe. <i>Chemistry of Materials</i> , 2016, 28, 3218-3226.	3.2	129
86	Concerted Rattling in CsAg ₅ Te ₃ Leading to Ultralow Thermal Conductivity and High Thermoelectric Performance. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 11431-11436.	7.2	144
87	Concerted Rattling in CsAg ₅ Te ₃ Leading to Ultralow Thermal Conductivity and High Thermoelectric Performance. <i>Angewandte Chemie</i> , 2016, 128, 11603-11608.	1.6	28
88	Ultralow Thermal Conductivity in Full Heusler Semiconductors. <i>Physical Review Letters</i> , 2016, 117, 046602.	2.9	163
89	Organic Dye Graphene Hybrid Structures with Spectral Color Selectivity. <i>Advanced Functional Materials</i> , 2016, 26, 6593-6600.	7.8	31
90	Structure and Failure Mechanism of the Thermoelectric CoSb ₃ /TiCoSb Interface. <i>ACS Applied Materials & Interfaces</i> , 2016, 8, 31968-31977.	4.0	13

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91	Non-equilibrium processing leads to record high thermoelectric figure of merit in PbTe/SrTe. Nature Communications, 2016, 7, 12167.	5.8	498
92	Au@MoS ₂ Core-Shell Heterostructures with Strong Light-Matter Interactions. Nano Letters, 2016, 16, 7696-7702.	4.5	139
93	Ultrahigh power factor and thermoelectric performance in hole-doped single-crystal SnSe. Science, 2016, 351, 141-144.	6.0	1,594
94	Lithium transport through lithium-ion battery cathode coatings. Journal of Materials Chemistry A, 2015, 3, 17248-17272.	5.2	109
95	Codoping in SnTe: Enhancement of Thermoelectric Performance through Synergy of Resonance Levels and Band Convergence. Journal of the American Chemical Society, 2015, 137, 5100-5112.	6.6	394
96	Valence Band Modification and High Thermoelectric Performance in SnTe Heavily Alloyed with MnTe. Journal of the American Chemical Society, 2015, 137, 11507-11516.	6.6	371
97	Theoretical Prediction and Experimental Confirmation of Unusual Ternary Ordered Semiconductor Compounds in Sr/Pb/S System. Journal of the American Chemical Society, 2014, 136, 1628-1635.	6.6	33
98	Origin of the High Performance in GeTe-Based Thermoelectric Materials upon Bi ₂ Te ₃ Doping. Journal of the American Chemical Society, 2014, 136, 11412-11419.	6.6	319
99	High Thermoelectric Performance via Hierarchical Compositionally Alloyed Nanostructures. Journal of the American Chemical Society, 2013, 135, 7364-7370.	6.6	344
100	Lithium Transport in Amorphous Al ₂ O ₃ and AlF ₃ for Discovery of Battery Coatings. Journal of Physical Chemistry C, 2013, 117, 8009-8013.	1.5	101
101	Raising the Thermoelectric Performance of p-Type PbS with Endotaxial Nanostructuring and Valence-Band Offset Engineering Using CdS and ZnS. Journal of the American Chemical Society, 2012, 134, 16327-16336.	6.6	308