Shiqiang Hao

List of Publications by Year
in descending order

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101 papers	8,764 citations	66234 42 h-index	43802 91 g-index
102 all docs	102 docs citations	102 times ranked	7004 citing authors

#	Article	IF	Citations
1	Thermoelectric Performance of the 2D Bi₂Si₂Te₆ Semiconductor. Journal of the American Chemical Society, 2022, 144, 1445-1454.	6.6	37
2	Extraordinary role of Zn in enhancing thermoelectric performance of Ga-doped n-type PbTe. Energy and Environmental Science, 2022, 15, 368-375.	15.6	107
3	Weak-Bonding Elements Lead to High Thermoelectric Performance in BaSnS₃ and SrSnS₃: A First-Principles Study. Chemistry of Materials, 2022, 34, 1289-1301.	3.2	19
4	Synergistic defect- and interfacial-engineering of a Bi₂S₃-based nanoplate network for high-performance photoelectrochemical solar water splitting. Journal of Materials Chemistry A, 2022, 10, 7830-7840.	5.2	13
5	Valence Disproportionation of GeS in the PbS Matrix Forms Pb₅Ge₅S₁₂ Inclusions with Conduction Band Alignment Leading to High n-Type Thermoelectric Performance. Journal of the American Chemical Society, 2022, 144, 7402-7413.	6.6	24
6	High Thermoelectric Performance in Chalcopyrite Cu_{1â€“x}Ag_xGaTe₂â€“ZnTe: Nontrivial Band Structure and Dynamic Doping Effect. Journal of the American Chemical Society, 2022, 144, 9113-9125.	6.6	29
7	Antimony doping to enhance luminescence of tin(<scp>iv</scp>)-based hybrid metal halides. Inorganic Chemistry Frontiers, 2022, 9, 3865-3873.	3.0	9
8	Probing the Optical Response and Local Dielectric Function of an Unconventional Si@MoS₂ Coreâ€“Shell Architecture. Nano Letters, 2022, 22, 4848-4853.	4.5	2
9	In₄Pb_{5.5}Sb₅S₁₉: A Stable Quaternary Chalcogenide with Low Thermal Conductivity. Inorganic Chemistry, 2021, 60, 325-333.	1.9	5
10	Strong Valence Band Convergence to Enhance Thermoelectric Performance in PbSe with Two Chemically Independent Controls. Angewandte Chemie, 2021, 133, 272-277.	1.6	7
11	Strong Valence Band Convergence to Enhance Thermoelectric Performance in PbSe with Two Chemically Independent Controls. Angewandte Chemie - International Edition, 2021, 60, 268-273.	7.2	28
12	Raspberry-like mesoporous Co-doped TiO₂ nanospheres for a high-performance formaldehyde gas sensor. Journal of Materials Chemistry A, 2021, 9, 6529-6537.	5.2	33
13	Sn_{4â^Î´}B₁₂Se₁₂[Q_x], Q = Se, Te, a B₁₂ Cluster Tunnel Framework Hosting Neutral Chalcogen Chains. Chemistry of Materials, 2021, 33, 1723-1730.	3.2	6
14	Dissociation of GaSb in n-Type PbTe: off-Centered Gallium Atom and Weak Electronâ€“Phonon Coupling Provide High Thermoelectric Performance. Chemistry of Materials, 2021, 33, 1842-1851.	3.2	23
15	Lithium Thiostannate Spinels: Air-Stable Cubic Semiconductors. Chemistry of Materials, 2021, 33, 2080-2089.	3.2	6
16	Implications of doping on microstructure, processing, and thermoelectric performance: The case of PbSe. Journal of Materials Research, 2021, 36, 1272-1284.	1.2	8
17	Ultralow Thermal Conductivity in Diamondoid Structures and High Thermoelectric Performance in (Cu_{1â€“x}Ag_x)(In_{1â€“y}Ga_y)Te₂ Journal of the American Chemical Society, 2021, 143, 5978-5989.	6.6	49
18	Vast Structural and Polymorphic Varieties of Semiconductors AMMâ€²Q4 (A = K, Rb, Cs, Tl; M = Ga, In; Mâ€² =) Tj ETQq0 0 0 rgBT /Over	3.2	6

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19	Broad Photoluminescence and Second-Harmonic Generation in the Noncentrosymmetric Organicâ€“Inorganic Hybrid Halide (C₆H₅(CH₂)₄NH₃)₄MX₇·H₂ (M = Bi, In, X = Br or I). Chemistry of Materials, 2021, 33, 8106-8111.	3.2	36
20	Structure Tuning, Strong Second Harmonic Generation Response, and High Optical Stability of the Polar Semiconductors Na_{1â€“x}K_xAsQ₂. Journal of the American Chemical Society, 2021, 143, 18204-18215.	6.6	24
21	Broadband light emitting zero-dimensional antimony and bismuth-based hybrid halides with diverse structures. Journal of Materials Chemistry C, 2021, 9, 15942-15948.	2.7	18
22	Decreasing Structural Dimensionality of Double Perovskites for Phase Stabilization toward Efficient X-ray Detection. ACS Applied Materials & Interfaces, 2021, 13, 61447-61453.	4.0	11
23	Optical phonon dominated heat transport: A first-principles thermal conductivity study of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BaSnS</mml:mi><mml:mn>2</mml:mn></mml:msub></m Physical Review B, 2021, 104, .	3.7	28
24	Discordant nature of Cd in PbSe: off-centering and coreâ€“shell nanoscale CdSe precipitates lead to high thermoelectric performance. Energy and Environmental Science, 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. Journal of Materials Chemistry A, 2020, 8, 1193-1204.	5.2	83
26	High-Performance Thermoelectrics from Cellular Nanostructured Sb2Si2Te6. Joule, 2020, 4, 159-175.	11.7	103
27	Superior Oxygen Reduction Reaction on Phosphorusâ€Doped Carbon Dot/Graphene Aerogel for Allâ€Solidâ€State Flexible Alâ€“Air Batteries. Advanced Energy Materials, 2020, 10, 1902736.	10.2	93
28	High Thermoelectric Performance in the New Cubic Semiconductor AgSnSbSe₃ by High-Entropy Engineering. Journal of the American Chemical Society, 2020, 142, 15187-15198.	6.6	108
29	Layered and Cubic Semiconductors AGaMâ€²Q₄ (A⁺ =) Tj ETQq1 1 0.784314 r gB High Third-Harmonic Generation. Journal of the American Chemical Society, 2020, 142, 17730-17742.	6.6	21
30	Ultralow thermal conductivity in diamondoid lattices: high thermoelectric performance in chalcopyrite Cu_{0.8+y}Ag_{0.2}In_{1â^'y}Te₂. Energy and Environmental Science, 2020, 13, 3693-3705.	15.6	52
31	Identifying the Origins of High Thermoelectric Performance in Group IIIA Element Doped PbS. ACS Applied Materials & Interfaces, 2020, 12, 14203-14212.	4.0	12
32	Crystal structure and luminescence properties of lead-free metal halides (C₆H₅CH₂NH₃)₃MBr₆ (M = Bi) Tj ETQq0 0 0 rgBT /Overl	2.7	6
33	Ultralow Thermal Conductivity and Thermoelectric Properties of Rb2Bi8Se13. Chemistry of Materials, 2020, 32, 3561-3569.	3.2	23
34	Direct Visualization of Electric-Field-Induced Structural Dynamics in Monolayer Transition Metal Dichalcogenides. ACS Nano, 2020, 14, 1569-1576.	7.3	23
35	All-Inorganic Halide Perovskites as Potential Thermoelectric Materials: Dynamic Cation off-Centering Induces Ultralow Thermal Conductivity. Journal of the American Chemical Society, 2020, 142, 9553-9563.	6.6	155
36	Topology of transition metal dichalcogenides: the case of the coreâ€“shell architecture. Nanoscale, 2020, 12, 23897-23919.	2.8	14

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37	Quasilinear dispersion in electronic band structure and high Seebeck coefficient in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>CuFe</mml:mi><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> -based thermoelectric materials. Physical Review Materials, 2020, 4, .	0.9	7
38	Ion Beam Induced Artifacts in Lead Based Chalcogenides. Microscopy and Microanalysis, 2019, 25, 2262-2263.	0.2	1
39	Ultralow Thermal Conductivity and High-Temperature Thermoelectric Performance in n-Type K_{2.5}Bi_{8.5}Se₁₄. Chemistry of Materials, 2019, 31, 5943-5952.	3.2	25
40	Large Thermal Conductivity Drops in the Diamondoid Lattice of CuFeS₂ by Discordant Atom Doping. Journal of the American Chemical Society, 2019, 141, 18900-18909.	6.6	66
41	Lead-Free Broadband Orange-Emitting Zero-Dimensional Hybrid (PMA)₃InBr₆ with Direct Band Gap. Inorganic Chemistry, 2019, 58, 15602-15609.	1.9	81
42	High Figure of Merit in Gallium-Doped Nanostructured n-Type PbTe-xGeTe with Midgap States. Journal of the American Chemical Society, 2019, 141, 16169-16177.	6.6	76
43	MoS2-capped CuxS nanocrystals: a new heterostructured geometry of transition metal dichalcogenides for broadband optoelectronics. Materials Horizons, 2019, 6, 587-594.	6.4	18
44	Origin of Intrinsically Low Thermal Conductivity in Talnakhite Cu_{17.6}Fe_{17.6}S₃₂ Thermoelectric Material: Correlations between Lattice Dynamics and Thermal Transport. Journal of the American Chemical Society, 2019, 141, 10905-10914.	6.6	50
45	Ion Beam Induced Artifacts in Lead-Based Chalcogenides. Microscopy and Microanalysis, 2019, 25, 831-839.	0.2	6
46	Computational strategies for design and discovery of nanostructured thermoelectrics. Npj Computational Materials, 2019, 5, .	3.5	39
47	Design Strategy for High-Performance Thermoelectric Materials: The Prediction of Electron-Doped KZrCuSe₃. Chemistry of Materials, 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. Journal of the American Chemical Society, 2019, 141, 6403-6412.	6.6	67
49	Six Quaternary Chalcogenides of the Pavonite Homologous Series with Ultralow Lattice Thermal Conductivity. Chemistry of Materials, 2019, 31, 3430-3439.	3.2	28
50	Enhanced Density-of-States Effective Mass and Strained Endotaxial Nanostructures in Sb-Doped Pb_{0.97}Cd_{0.03}Te Thermoelectric Alloys. ACS Applied Materials & Interfaces, 2019, 11, 9197-9204.	4.0	66
51	Probing Strain-Induced Band Gap Modulation in 2D Hybrid Organicâ€“Inorganic Perovskites. ACS Energy Letters, 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. Journal of the American Chemical Society, 2019, 141, 4480-4486.	6.6	87
53	Thermoelectric Material SnPb2Bi2S6: The 4,4L Member of Lillianite Homologous Series with Low Lattice Thermal Conductivity. Inorganic Chemistry, 2019, 58, 1339-1348.	1.9	10
54	High Thermoelectric Performance in the Wide Bandâ€Gap AgGa_{1â€}_xTe₂ Compounds: Directional Negative Thermal Expansion and Intrinsically Low Thermal Conductivity. Advanced Functional Materials, 2019, 29, 1806534.	7.8	65

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55	Computational prediction of nanostructured alloys with enhanced thermoelectric properties. Physical Review Materials, 2019, 3, .	0.9	3
56	Dimensionally driven crossover from semimetal to direct semiconductor in layered SbAs. Physical Review Materials, 2019, 3, .	0.9	1
57	Intrinsic Transport in 2D Heterostructures Mediated through h-BN Tunneling Contacts. Nano Letters, 2018, 18, 2990-2998.	4.5	39
58	First-Principles Study of Lithium Cobalt Spinel Oxides: Correlating Structure and Electrochemistry. ACS Applied Materials & Interfaces, 2018, 10, 13479-13490.	4.0	31
59	Optically Active 1D MoS₂ Nanobelts. ACS Applied Materials & Interfaces, 2018, 10, 6799-6804.	4.0	23
60	High Thermoelectric Performance in SnTeâ€“AgSbTe₂ Alloys from Lattice Softening, Giant Phononâ€“Vacancy Scattering, and Valence Band Convergence. ACS Energy Letters, 2018, 3, 705-712.	8.8	151
61	Largeâ€Scale Fabrication of MoS₂ Ribbons and Their Lightâ€Induced Electronic/Thermal Properties: Dichotomies in the Structural and Defect Engineering. Advanced Functional Materials, 2018, 28, 1704863.	7.8	25
62	Quaternary Pavonites A_{1+x}Sn_{2â€“x}Bi_{5+x}S₁₀ (A⁺ = Li⁺, Na⁺): Site Occupancy Disorder Defines Electronic Structure. Inorganic Chemistry, 2018, 57, 2260-2268.	1.9	12
63	Grain Boundaries Softening Thermoelectric Oxide BiCuSeO. ACS Applied Materials & Interfaces, 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. Journal of the American Chemical Society, 2018, 140, 2673-2686.	6.6	307
65	High thermoelectric performance in Bi_{0.46}Sb_{1.54}Te₃ nanostructured with ZnTe. Energy and Environmental Science, 2018, 11, 1520-1535.	15.6	239
66	nâ€Type SnSe₂ Orientedâ€Nanoplateâ€Based Pellets for High Thermoelectric Performance. Advanced Energy Materials, 2018, 8, 1702167.	10.2	103
67	First-principles calculations and experimental studies of XYZ₂ thermoelectric compounds: detailed analysis of van der Waals interactions. Journal of Materials Chemistry A, 2018, 6, 19502-19519.	5.2	20
68	Chemical Insights into PbSeâ€“x%HgSe: High Power Factor and Improved Thermoelectric Performance by Alloying with Discordant Atoms. Journal of the American Chemical Society, 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. ACS Energy Letters, 2018, 3, 2593-2601.	8.8	37
70	Weak Electron Phonon Coupling and Deep Level Impurity for High Thermoelectric Performance Pb_{1â^’}_xGa_xTe. Advanced Energy Materials, 2018, 8, 1800659.	10.2	111
71	Absence of Nanostructuring in NaPb_mSbTe_{m+2}: Solid Solutions with High Thermoelectric Performance in the Intermediate Temperature Regime. Journal of the American Chemical Society, 2018, 140, 7021-7031.	6.6	27
72	Quaternary Chalcogenide Semiconductors with 2D Structures: Rb2ZnBi2Se5 and Cs6Cd2Bi8Te17. Inorganic Chemistry, 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. Journal of Materials Chemistry A, 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 PbSeâ€“GeSe. Energy and Environmental Science, 2018, 11, 3220-3230.	15.6	115
75	The New Semiconductor Cs₄Cu₃Bi₉S₁₇. Chemistry of Materials, 2017, 29, 1744-1751.	3.2	13
76	Systematic Study of Oxygen Vacancy Tunable Transport Properties of Fewâ€Layer MoO<sub>3â<sub>_x Enabled by Vaporâ€Based Synthesis. Advanced Functional Materials, 2017, 27, 1605380.	7.8	91
77	High Thermoelectric Performance in Electron-Doped AgBi₃S₅ with Ultralow Thermal Conductivity. Journal of the American Chemical Society, 2017, 139, 6467-6473.	6.6	160
78	Bi₂PdO₄: A Promising Thermoelectric Oxide with High Power Factor and Low Lattice Thermal Conductivity. Chemistry of Materials, 2017, 29, 2529-2534.	3.2	42
79	In-situ Electron Diffraction Studies of Sodium Electrochemistry in MoS2. Microscopy and Microanalysis, 2017, 23, 2050-2051.	0.2	0
80	Homologous Series of 2D Chalcogenides Csâ€“Agâ€“Biâ€“Q (Q = S, Se) with Ion-Exchange Properties. Journal of the American Chemical Society, 2017, 139, 12601-12609.	6.6	22
81	Pressure induced thermoelectric enhancement in SnSe crystals. Journal of Materials Chemistry A, 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. Microscopy and Microanalysis, 2016, 22, 1268-1269.	0.2	0
83	High-throughput computational design of cathode coatings for Li-ion batteries. Nature Communications, 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. APL Materials, 2016, 4, .	2.2	29
85	Computational Prediction of High Thermoelectric Performance in Hole Doped Layered GeSe. Chemistry of Materials, 2016, 28, 3218-3226.	3.2	129
86	Concerted Rattling in CsAg₅Te₃ Leading to Ultralow Thermal Conductivity and High Thermoelectric Performance. Angewandte Chemie - International Edition, 2016, 55, 11431-11436.	7.2	144
87	Concerted Rattling in CsAg₅Te₃ Leading to Ultralow Thermal Conductivity and High Thermoelectric Performance. Angewandte Chemie, 2016, 128, 11603-11608.	1.6	28
88	Ultralow Thermal Conductivity in Full Heusler Semiconductors. Physical Review Letters, 2016, 117, 046602.	2.9	163
89	Organic Dye Graphene Hybrid Structures with Spectral Color Selectivity. Advanced Functional Materials, 2016, 26, 6593-6600.	7.8	31
90	Structure and Failure Mechanism of the Thermoelectric CoSb₃/TiCoSb Interface. ACS Applied Materials & Interfaces, 2016, 8, 31968-31977.	4.0	13

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91	Non-equilibrium processing leads to record high thermoelectric figure of merit in PbTeâ€“SrTe. Nature Communications, 2016, 7, 12167.	5.8	498
92	Au@MoS₂ Coreâ€“Shell Heterostructures with Strong Lightâ€“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 Srâ€“Pbâ€“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 Bi₂Te₃ 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 Al₂O₃ and AlF₃ 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