Shiqiang Hao

List of Publications by Year
in descending order

101 papers	8,764 citations	66315 42 h-index	42364 92 g-index
102 all docs	102 docs citations	102 times ranked	7004 citing authors

#	Article	IF	Citations
1	Ultrahigh power factor and thermoelectric performance in hole-doped single-crystal SnSe. Science, 2016, 351, 141-144.	6.0	1,594
2	Non-equilibrium processing leads to record high thermoelectric figure of merit in PbTeâ€“SrTe. Nature Communications, 2016, 7, 12167.	5.8	498
3	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
4	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
5	High Thermoelectric Performance via Hierarchical Compositionally Alloyed Nanostructures. Journal of the American Chemical Society, 2013, 135, 7364-7370.	6.6	344
6	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
7	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
8	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
9	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
10	Ultralow Thermal Conductivity in Full Heusler Semiconductors. Physical Review Letters, 2016, 117, 046602.	2.9	163
11	High Thermoelectric Performance in Electron-Doped AgBi₃S₅ with Ultralow Thermal Conductivity. Journal of the American Chemical Society, 2017, 139, 6467-6473.	6.6	160
12	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
13	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
14	High-throughput computational design of cathode coatings for Li-ion batteries. Nature Communications, 2016, 7, 13779.	5.8	145
15	Concerted Rattling in CsAg₅Te₃ Leading to Ultralow Thermal Conductivity and High Thermoelectric Performance. Angewandte Chemie - International Edition, 2016, 55, 11431-11436.	7.2	144
16	Au@MoS₂ Coreâ€“Shell Heterostructures with Strong Lightâ€“Matter Interactions. Nano Letters, 2016, 16, 7696-7702.	4.5	139
17	Computational Prediction of High Thermoelectric Performance in Hole Doped Layered GeSe. Chemistry of Materials, 2016, 28, 3218-3226.	3.2	129
18	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

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19	Weak Electron Phonon Coupling and Deep Level Impurity for High Thermoelectric Performance Pb_{1â^'}<i>_x</i>Ga<i>_x</i>Te. Advanced Energy Materials, 2018, 8, 1800659.	10.2	111
20	Lithium transport through lithium-ion battery cathode coatings. Journal of Materials Chemistry A, 2015, 3, 17248-17272.	5.2	109
21	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
22	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
23	nâ€Type SnSe₂ Orientedâ€Nanoplateâ€Based Pellets for High Thermoelectric Performance. Advanced Energy Materials, 2018, 8, 1702167.	10.2	103
24	High-Performance Thermoelectrics from Cellular Nanostructured Sb2Si2Te6. Joule, 2020, 4, 159-175.	11.7	103
25	Lithium Transport in Amorphous Al₂O₃ and AlF₃ for Discovery of Battery Coatings. Journal of Physical Chemistry C, 2013, 117, 8009-8013.	1.5	101
26	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
27	Systematic Study of Oxygen Vacancy Tunable Transport Properties of Fewâ€Layer MoO_{3â^'}<i>_x</i> Enabled by Vaporâ€Based Synthesis. Advanced Functional Materials, 2017, 27, 1605380.	7.8	91
28	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
29	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
30	Pressure induced thermoelectric enhancement in SnSe crystals. Journal of Materials Chemistry A, 2016, 4, 12073-12079.	5.2	81
31	Lead-Free Broadband Orange-Emitting Zero-Dimensional Hybrid (PMA)₃InBr₆ with Direct Band Gap. Inorganic Chemistry, 2019, 58, 15602-15609.	1.9	81
32	Chemical Insights into PbSeâ€"<i>x</i>%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
33	High Figure of Merit in Gallium-Doped Nanostructured n-Type PbTe-<i>x</i>GeTe with Midgap States. Journal of the American Chemical Society, 2019, 141, 16169-16177.	6.6	76
34	Crystal structure and luminescence properties of lead-free metal halides (C₆H₅CH₂NH₃)₃MBr₆ (M = Bi) Tj ET Q q 0 0 0 rg BT /Overl	2.7	69
35	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
36	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

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37	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
38	High Thermoelectric Performance in the Wide Bandâ€Gap AgGa_{1â€}<i>_x</i>Te₂ Compounds: Directional Negative Thermal Expansion and Intrinsically Low Thermal Conductivity. Advanced Functional Materials, 2019, 29, 1806534.	7.8	65
39	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
40	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
41	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
42	Ultralow Thermal Conductivity in Diamondoid Structures and High Thermoelectric Performance in (Cu_{1â€"<i>x</i>}Ag_{<i>x</i>})(In_{1â€"<i>y</i>}Ga_{<i>y</i>})Te₂. Journal of the American Chemical Society, 2021, 143, 5978-5989.	6.6	49
43	Probing Strain-Induced Band Gap Modulation in 2D Hybrid Organicâ€"Inorganic Perovskites. ACS Energy Letters, 2019, 4, 796-802.	8.8	47
44	Bi₂PdO₄: A Promising Thermoelectric Oxide with High Power Factor and Low Lattice Thermal Conductivity. Chemistry of Materials, 2017, 29, 2529-2534.	3.2	42
45	Intrinsic Transport in 2D Heterostructures Mediated through h-BN Tunneling Contacts. Nano Letters, 2018, 18, 2990-2998.	4.5	39
46	Computational strategies for design and discovery of nanostructured thermoelectrics. Npj Computational Materials, 2019, 5, .	3.5	39
47	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
48	Thermoelectric Performance of the 2D Bi₂Si₂Te₆ Semiconductor. Journal of the American Chemical Society, 2022, 144, 1445-1454.	6.6	37
49	Broad Photoluminescence and Second-Harmonic Generation in the Noncentrosymmetric Organicâ€"Inorganic Hybrid Halide (C₆H₅(CH₂)₄NH₃)₄MX₇Â·H<sub>2</sub (M = Bi, In, X = Br or I). Chemistry of Materials, 2021, 33, 8106-8111.	3.2	36
50	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
51	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
52	Organic Dye Graphene Hybrid Structures with Spectral Color Selectivity. Advanced Functional Materials, 2016, 26, 6593-6600.	7.8	31
53	First-Principles Study of Lithium Cobalt Spinel Oxides: Correlating Structure and Electrochemistry. ACS Applied Materials & Interfaces, 2018, 10, 13479-13490.	4.0	31
54	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

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55	High Thermoelectric Performance in Chalcopyrite Cu_{1â€“<i>x</i>}Ag_{<i>x</i>}GaTe₂â€“ZnTe: Nontrivial Band Structure and Dynamic Doping Effect. Journal of the American Chemical Society, 2022, 144, 9113-9125.	6.6	29
56	Concerted Rattling in CsAg₅Te₃ Leading to Ultralow Thermal Conductivity and High Thermoelectric Performance. Angewandte Chemie, 2016, 128, 11603-11608.	1.6	28
57	Six Quaternary Chalcogenides of the Pavonite Homologous Series with Ultralow Lattice Thermal Conductivity. Chemistry of Materials, 2019, 31, 3430-3439.	3.2	28
58	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
59	Absence of Nanostructuring in NaPb_{<i>m</i>}SbTe_{<i>m</i>+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
60	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
61	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
62	Structure Tuning, Strong Second Harmonic Generation Response, and High Optical Stability of the Polar Semiconductors Na_{1â€“<i>x</i>}K_{<i>x</i>}As<i>Q</i>₂. Journal of the American Chemical Society, 2021, 143, 18204-18215.	6.6	24
63	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
64	Optically Active 1D MoS₂ Nanobelts. ACS Applied Materials & Interfaces, 2018, 10, 6799-6804.	4.0	23
65	Design Strategy for High-Performance Thermoelectric Materials: The Prediction of Electron-Doped KZrCuSe₃. Chemistry of Materials, 2019, 31, 3018-3024.	3.2	23
66	Ultralow Thermal Conductivity and Thermoelectric Properties of Rb2Bi8Se13. Chemistry of Materials, 2020, 32, 3561-3569.	3.2	23
67	Direct Visualization of Electric-Field-Induced Structural Dynamics in Monolayer Transition Metal Dichalcogenides. ACS Nano, 2020, 14, 1569-1576.	7.3	23
68	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
69	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>< Physical Review B, 2021, 104, .	1.1	23
70	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
71	Layered and Cubic Semiconductors <i>A</i>Ga<i>M</i>â€²<i>Q</i>₄ (<i>A</i>⁺ =) Tj ETQq1 1 0.784314 rgB High Third-Harmonic Generation. Journal of the American Chemical Society, 2020, 142, 17730-17742.	6.6	21
72	First-principles calculations and experimental studies of <i>XYZ</i>₂ thermoelectric compounds: detailed analysis of van der Waals interactions. Journal of Materials Chemistry A, 2018, 6, 19502-19519.	5.2	20

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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	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
75	MoS2-capped CuxS nanocrystals: a new heterostructured geometry of transition metal dichalcogenides for broadband optoelectronics. Materials Horizons, 2019, 6, 587-594.	6.4	18
76	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
77	Topology of transition metal dichalcogenides: the case of the coreâ€“shell architecture. Nanoscale, 2020, 12, 23897-23919.	2.8	14
78	Structure and Failure Mechanism of the Thermoelectric CoSb₃/TiCoSb Interface. ACS Applied Materials & Interfaces, 2016, 8, 31968-31977.	4.0	13
79	The New Semiconductor Cs₄Cu₃Bi₉S₁₇. Chemistry of Materials, 2017, 29, 1744-1751.	3.2	13
80	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
81	Quaternary Pavonites A_{1+<i>x</i>}Sn_{2â€“<i>x</i>}Bi_{5+<i>x</i>}S₁₀ (A⁺ = Li⁺, Na⁺): Site Occupancy Disorder Defines Electronic Structure. Inorganic Chemistry, 2018, 57, 2260-2268.	1.9	12
82	Identifying the Origins of High Thermoelectric Performance in Group IIIA Element Doped PbS. ACS Applied Materials & Interfaces, 2020, 12, 14203-14212.	4.0	12
83	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
84	Grain Boundaries Softening Thermoelectric Oxide BiCuSeO. ACS Applied Materials & Interfaces, 2018, 10, 6772-6777.	4.0	10
85	Quaternary Chalcogenide Semiconductors with 2D Structures: Rb2ZnBi2Se5 and Cs6Cd2Bi8Te17. Inorganic Chemistry, 2018, 57, 9403-9411.	1.9	10
86	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
87	Antimony doping to enhance luminescence of tin(<scp>iv</scp>)-based hybrid metal halides. Inorganic Chemistry Frontiers, 2022, 9, 3865-3873.	3.0	9
88	Implications of doping on microstructure, processing, and thermoelectric performance: The case of PbSe. Journal of Materials Research, 2021, 36, 1272-1284.	1.2	8
89	Strong Valence Band Convergence to Enhance Thermoelectric Performance in PbSe with Two Chemically Independent Controls. Angewandte Chemie, 2021, 133, 272-277.	1.6	7
90	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

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91	Ion Beam Induced Artifacts in Lead-Based Chalcogenides. Microscopy and Microanalysis, 2019, 25, 831-839.	0.2	6
92	Sn_{4â`Î´}B₁₂Se₁₂[Q_{<i>x</i>}], Q = Se, Te, a B₁₂ Cluster Tunnel Framework Hosting Neutral Chalcogen Chains. Chemistry of Materials, 2021, 33, 1723-1730.	3.2	6
93	Lithium Thiostannate Spinels: Air-Stable Cubic Semiconductors. Chemistry of Materials, 2021, 33, 2080-2089.	3.2	6
94	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
95	In₄Pb_{5.5}Sb₅S₁₉: A Stable Quaternary Chalcogenide with Low Thermal Conductivity. Inorganic Chemistry, 2021, 60, 325-333.	1.9	5
96	Computational prediction of nanostructured alloys with enhanced thermoelectric properties. Physical Review Materials, 2019, 3, .	0.9	3
97	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
98	Ion Beam Induced Artifacts in Lead Based Chalcogenides. Microscopy and Microanalysis, 2019, 25, 2262-2263.	0.2	1
99	Dimensionally driven crossover from semimetal to direct semiconductor in layered SbAs. Physical Review Materials, 2019, 3, .	0.9	1
100	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
101	In-situ Electron Diffraction Studies of Sodium Electrochemistry in MoS2. Microscopy and Microanalysis, 2017, 23, 2050-2051.	0.2	0