Wenqing Zhang

List of Publications by Year
in descending order

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78 papers	7,457 citations	126907 33 h-index	66911 78 g-index
80 all docs	80 docs citations	80 times ranked	6572 citing authors

#	Article	IF	Citations
1	Copper ion liquid-like thermoelectrics. Nature Materials, 2012, 11, 422-425.	27.5	1,700
2	Multiple-Filled Skutterudites: High Thermoelectric Figure of Merit through Separately Optimizing Electrical and Thermal Transports. Journal of the American Chemical Society, 2011, 133, 7837-7846.	13.7	1,242
3	On the tuning of electrical and thermal transport in thermoelectrics: an integrated theoryâ€“experiment perspective. Npj Computational Materials, 2016, 2, .	8.7	399
4	Giant thermopower of ionic gelatin near room temperature. Science, 2020, 368, 1091-1098.	12.6	382
5	The role of the solid electrolyte interphase layer in preventing Li dendrite growth in solid-state batteries. Energy and Environmental Science, 2018, 11, 1803-1810.	30.8	304
6	Part-crystalline part-liquid state and rattling-like thermal damping in materials with chemical-bond hierarchy. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 15031-15035.	7.1	225
7	Reaction Mechanisms for Long-Life Rechargeable Zn/MnO₂ Batteries. Chemistry of Materials, 2019, 31, 2036-2047.	6.7	195
8	Cuâ”Se Bond Network and Thermoelectric Compounds with Complex Diamondlike Structure. Chemistry of Materials, 2010, 22, 6029-6031.	6.7	189
9	High intrinsic carrier mobility and photon absorption in the perovskite CH₃NH₃PbI₃. Physical Chemistry Chemical Physics, 2015, 17, 11516-11520.	2.8	182
10	Boosting the thermoelectric performance of PbSe through dynamic doping and hierarchical phonon scattering. Energy and Environmental Science, 2018, 11, 1848-1858.	30.8	163
11	Suppression of atom motion and metal deposition in mixed ionic electronic conductors. Nature Communications, 2018, 9, 2910.	12.8	148
12	Complex Band Structures and Lattice Dynamics of Bi₂Te₃â€Based Compounds and Solid Solutions. Advanced Functional Materials, 2019, 29, 1900677.	14.9	135
13	Discovery of High-Performance Thermoelectric Chalcogenides through Reliable High-Throughput Material Screening. Journal of the American Chemical Society, 2018, 140, 10785-10793.	13.7	134
14	Realization of higher thermoelectric performance by dynamic doping of copper in n-type PbTe. Energy and Environmental Science, 2019, 12, 3089-3098.	30.8	127
15	Semiconductor glass with superior flexibility and high room temperature thermoelectric performance. Science Advances, 2020, 6, eaaz8423.	10.3	108
16	Simplified Synthesis of Fluoride-Free Ti₃C₂T_x via Electrochemical Etching toward High-Performance Electrochemical Capacitors. ACS Nano, 2022, 16, 2461-2470.	14.6	99
17	Mg₃₊_{Î´}Sb_xBi_{2â”}_x Family: A Promising Substitute for the Stateâ€ofâ€theâ€Art nâ€Type Thermoelectric Materials near Room Temperature. Advanced Functional Materials, 2019, 29, 1807235.	14.9	98
18	High-throughput screening platform for solid electrolytes combining hierarchical ion-transport prediction algorithms. Scientific Data, 2020, 7, 151.	5.3	90

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19	Short-range order in defective half-Heusler thermoelectric crystals. Energy and Environmental Science, 2019, 12, 1568-1574.	30.8	86
20	Two-dimensional thermoelectrics with Rashba spin-split bands in bulk BiTeI. Physical Review B, 2014, 90, .	3.2	74
21	High-Throughput Screening for Advanced Thermoelectric Materials: Diamond-Like ABX₂ Compounds. ACS Applied Materials & Interfaces, 2019, 11, 24859-24866.	8.0	72
22	Achieving band convergence by tuning the bonding ionicity in nâ€type Mg₃Sb₂. Journal of Computational Chemistry, 2019, 40, 1693-1700.	3.3	68
23	Regulating Excitonâ€“Phonon Coupling to Achieve a Nearâ€Unity Photoluminescence Quantum Yield in Oneâ€Dimensional Hybrid Metal Halides. Advanced Science, 2021, 8, e2100786.	11.2	61
24	Rationalizing the interphase stability of Li|doped-Li₇La₃Zr₂O₁₂ via automated reaction screening and machine learning. Journal of Materials Chemistry A, 2019, 7, 19961-19969.	10.3	59
25	Mechanical Strainâ€Tunable Microwave Magnetism in Flexible CuFe₂O₄ Epitaxial Thin Film for Wearable Sensors. Advanced Functional Materials, 2018, 28, 1705928.	14.9	58
26	TransOpt. A code to solve electrical transport properties of semiconductors in constant electronâ€“phonon coupling approximation. Computational Materials Science, 2021, 186, 110074.	3.0	55
27	Theory for the Charge-Density-Wave Mechanism of 3D Quantum Hall Effect. Physical Review Letters, 2020, 125, 206601.	7.8	50
28	Active learning for the power factor prediction in diamond-like thermoelectric materials. Npj Computational Materials, 2020, 6, .	8.7	43
29	CAVD, towards better characterization of void space for ionic transport analysis. Scientific Data, 2020, 7, 153.	5.3	43
30	All solid thick oxide cathodes based on low temperature sintering for high energy solid batteries. Energy and Environmental Science, 2021, 14, 5044-5056.	30.8	41
31	Tuning Electrical Conductance in Bilayer MoS₂ through Defect-Mediated Interlayer Chemical Bonding. ACS Nano, 2020, 14, 10265-10275.	14.6	40
32	High Thermoelectric Performance through Crystal Symmetry Enhancement in Triply Doped Diamondoid Compound Cu₂SnSe₃. Advanced Energy Materials, 2021, 11, 2100661.	19.5	39
33	Boosting Transport Kinetics of Ions and Electrons Simultaneously by Ti3C2Tx (MXene) Addition for Enhanced Electrochromic Performance. Nano-Micro Letters, 2021, 13, 20.	27.0	37
34	Tuning colour centres at a twisted hexagonal boron nitride interface. Nature Materials, 2022, 21, 896-902.	27.5	31
35	Reducing the charge overpotential of Liâ€“O₂ batteries through band-alignment cathode design. Energy and Environmental Science, 2020, 13, 2540-2548.	30.8	30
36	Two-dimensional topological materials discovery by symmetry-indicator method. Physical Review B, 2019, 100, .	3.2	29

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37	The Electronic Transport Channel Protection and Tuning in Real Space to Boost the Thermoelectric Performance of Mg _{3+ Î´} Sb _{2- y} Bi _y near Room Temperature. Research, 2020, 2020, 1672051.	5.7	29
38	Large Transverse and Longitudinal Magnetoâ€Thermoelectric Effect in Polycrystalline Nodalâ€Line Semimetal Mg₃Bi₂. Advanced Materials, 2022, 34, e2200931.	21.0	28
39	Materials informatics platform with three dimensional structures, workflow and thermoelectric applications. Scientific Data, 2021, 8, 236.	5.3	27
40	A highly asymmetric interfacial superstructure in WC: expanding the classic grain boundary segregation and new complexion theories. Materials Horizons, 2020, 7, 173-180.	12.2	26
41	Violation of the T ^{â^'1} Relationship in the Lattice Thermal Conductivity of Mg ₃ Sb ₂ with Locally Asymmetric Vibrations. Research, 2020, 2020, 4589786.	5.7	25
42	Defect-mediated Rashba engineering for optimizing electrical transport in thermoelectric BiTeI. Npj Computational Materials, 2020, 6, .	8.7	24
43	Interfacial superstructures and chemical bonding transitions at metal-ceramic interfaces. Science Advances, 2021, 7, .	10.3	24
44	Generic Seebeck effect from spin entropy. Innovation(China), 2021, 2, 100101.	9.1	20
45	Half-Heusler-like compounds with wide continuous compositions and tunable p- to n-type semiconducting thermoelectrics. Nature Communications, 2022, 13, 35.	12.8	20
46	Electric Polarization Switching on an Atomically Thin Metallic Oxide. Nano Letters, 2021, 21, 144-150.	9.1	19
47	The variation of intrinsic defects in XTe (X = Ge, Sn, and Pb) induced by the energy positions of valence band maxima. Journal of Materials Chemistry C, 2021, 9, 5765-5770.	5.5	19
48	Thermal transport in thermoelectric materials with chemical bond hierarchy. Journal of Physics Condensed Matter, 2019, 31, 183002.	1.8	19
49	Prediction of protected band edge states and dielectric tunable quasiparticle and excitonic properties of monolayer MoSi2N4. Npj Computational Materials, 2022, 8, .	8.7	19
50	Thermopower enhancement in quantum wells with the Rashba effect. Applied Physics Letters, 2014, 105, .	3.3	18
51	A₂Cu₃In₃Te₈ (A = Cd, Zn, Mn, Mg): A Type of Thermoelectric Material with Complex Diamond-like Structure and Low Lattice Thermal Conductivities. ACS Applied Energy Materials, 2019, 2, 8956-8965.	5.1	17
52	Thermal transport in amorphous small organic materials: a mechanistic study. Physical Chemistry Chemical Physics, 2020, 22, 3058-3065.	2.8	16
53	Tetrahedral Distortion and Thermoelectric Performance of the Ag-Substituted CuInTe₂ Chalcopyrite Compound. ACS Applied Energy Materials, 2020, 3, 11015-11023.	5.1	16
54	Temperature-Dependent Band Renormalization in CoSb₃ Skutterudites Due to Sb-Ring-Related Vibrations. Chemistry of Materials, 2021, 33, 1046-1052.	6.7	16

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55	Flexible Ti₃C₂T_x/Nanocellulose Hybrid Film as a Stable Zn-free Anode for Aqueous Hybrid Znâ€“Li Batteries. ACS Applied Materials & Interfaces, 2022, 14, 6876-6884.	8.0	16
56	Thermodynamic Ground States of Multifunctional Metal Dodecaborides. Chemistry of Materials, 2019, 31, 1075-1083.	6.7	15
57	Prediction and Classification of Formation Energies of Binary Compounds by Machine Learning: An Approach without Crystal Structure Information. ACS Omega, 2021, 6, 14533-14541.	3.5	13
58	Sublattice Short-Range Order and Modified Electronic Structure in Defective Half-Heusler Nb_{0.8}CoSb. Journal of Physical Chemistry C, 2021, 125, 1125-1133.	3.1	13
59	5-IP7 is a GPCR messenger mediating neural control of synaptotagmin-dependent insulin exocytosis and glucose homeostasis. Nature Metabolism, 2021, 3, 1400-1414.	11.9	13
60	Temperatureâ€dependent structural fluctuation and its effect on the electronic structure and charge transport in hybrid perovskite <scp>CH₃NH₃PbI₃</scp>. Journal of Computational Chemistry, 2021, 42, 2213-2220.	3.3	12
61	Discovery of a Slaterâ€“Pauling Semiconductor ZrRu_{1.5}Sb with Promising Thermoelectric Properties. Advanced Functional Materials, 2022, 32, .	14.9	12
62	Solidâ€State Janus Nanoprecipitation Enables Amorphousâ€Like Heat Conduction in Crystalline Mg₃Sb₂â€Based Thermoelectric Materials. Advanced Science, 2022, 9, .	11.2	12
63	Enhanced Hardness in Transition-Metal Monocarbides via Optimal Occupancy of Bonding Orbitals. ACS Applied Materials & Interfaces, 2021, 13, 14365-14376.	8.0	11
64	Giant Narrow-Band Optical Absorption and Distinctive Excitonic Structures of Monolayer <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:mrow><mml:m	3.8	11
65	mathvariant="normal">N</mml:mi></mml:mrow></mml:mrow></mml:math> and <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">B</mml:mi></mml:mrow></mml:mrow><mml:mn>3</mml:mn></mml:msub><mml:mrow><mml:mrow><mml:mi mathvariant="normal">C</mml:mi></mml:mrow></mml:mrow></mml:math>. Physical Review Applied, 2020, 14, .	3.8	9
66	Dynamic process of the resonant phonon scattering in fully filled skutterudites. Physical Review B, 2018, 98, .	3.2	10
67	Crystal structures and formation mechanisms of boron-rich tungsten borides. Physical Review B, 2021, 104, .	3.2	10
68	Liquid-phase sintering enabling mixed ionic-electronic interphases and free-standing composite cathode architecture toward high energy solid-state battery. Nano Research, 2022, 15, 6156-6167.	10.4	10
69	Unraveling the relationships between chemical bonding and thermoelectric properties: n-type ABO₃ perovskites. Journal of Materials Chemistry A, 2022, 10, 11039-11045.	10.3	10
70	Remarkable Band-Gap Renormalization via Dimensionality of the Layered Material <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:mrow><mml:mrow><mml:mi mathvariant="normal">B</mml:mi></mml:mrow></mml:mrow></mml:mrow></mml:math>. Physical Review Applied, 2020, 14, .	3.8	9
71	Combined subsampling and analytical integration for efficient large-scale GW calculations for 2D systems. Npj Computational Materials, 2020, 6, .	8.7	9
72	Dual adaptive sampling and machine learning interatomic potentials for modeling materials with chemical bond hierarchy. Physical Review B, 2021, 104, .	3.2	9
	Localization in the SCAN meta-generalized gradient approximation functional leading to broken symmetry ground states for graphene and benzene. Physical Chemistry Chemical Physics, 2020, 22, 19585-19591.	2.8	8

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73	A general strategy for high-throughput experimental screening of promising bulk thermoelectric materials. Science China Materials, 2021, 64, 1751-1760.	6.3	8
74	Designing vacancy-filled Heusler thermoelectric semiconductors by the Slater-Pauling rule. Materials Today Energy, 2022, 27, 101035.	4.7	8
75	Isosymmetric phase transitions, ultrahigh ductility, and topological nodal lines in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Î±</mml:mi><mml:mo>â^'</mml:mo><mml:mi mathvariant="normal">A</mml:mi><mml:msub><mml:mi mathvariant="normal">g</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">S</mml:mi></mml:mrow></mml:math>. Physical Review B, 2020, 102, .	3.2	4
76	Flexible Electronics: Mechanical Strainâ€Tunable Microwave Magnetism in Flexible CuFe₂O₄ Epitaxial Thin Film for Wearable Sensors (Adv. Funct. Mater. 10/2018). Advanced Functional Materials, 2018, 28, 1870063.	14.9	3
77	Thermoelectrics: Mg₃₊_{Î´}Sb_xBi_{2â^'}_x Family: A Promising Substitute for the Stateâ€ofâ€theâ€Art nâ€Type Thermoelectric Materials near Room Temperature (Adv. Funct. Mater. 4/2019). Advanced Functional Materials, 2019, 29, 1970020.	14.9	2
78	Ag rearrangement induced metal-insulator phase transition in thermoelectric MgAgSb. Materials Today Physics, 2022, 25, 100702.	6.0	0