Ming Hu

List of Publications by Year
in descending order

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185 papers	7,601 citations	44069 48 h-index	64796 79 g-index
189 all docs	189 docs citations	189 times ranked	6662 citing authors

#	Article	IF	Citations
1	Anisotropic intrinsic lattice thermal conductivity of phosphorene from first principles. Physical Chemistry Chemical Physics, 2015, 17, 4854-4858.	2.8	379
2	Diverse anisotropy of phonon transport in two-dimensional group IVâ€“VI compounds: A comparative study. Nanoscale, 2016, 8, 11306-11319.	5.6	234
3	Thermal conductivity of silicene calculated using an optimized Stillinger-Weber potential. Physical Review B, 2014, 89, .	3.2	213
4	Hot-pressing induced alignment of boron nitride in polyurethane for composite films with thermal conductivity over 50â€¯Wmâ^'1â€¯Kâ^'1. Composites Science and Technology, 2018, 160, 199-207.	7.8	212
5	Significant Reduction of Thermal Conductivity in Si/Ge Coreâ^'Shell Nanowires. Nano Letters, 2011, 11, 618-623.	9.1	205
6	Si/Ge Superlattice Nanowires with Ultralow Thermal Conductivity. Nano Letters, 2012, 12, 5487-5494.	9.1	194
7	Disparate Strain Dependent Thermal Conductivity of Two-dimensional Penta-Structures. Nano Letters, 2016, 16, 3831-3842.	9.1	183
8	Anomalous thermal response of silicene to uniaxial stretching. Physical Review B, 2013, 87, .	3.2	179
9	Evaluating explorative prediction power of machine learning algorithms for materials discovery using<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:mrow><mml:mi>k</mml:mi></mml:mrow></mml:math>-fold forward cross-validation. Computational Materials Science, 2020, 171, 109203.	3.0	176
10	A facile method to prepare flexible boron nitride/poly(vinyl alcohol) composites with enhanced thermal conductivity. Composites Science and Technology, 2017, 149, 41-47.	7.8	170
11	Large tunability of lattice thermal conductivity of monolayer silicene via mechanical strain. Physical Review B, 2016, 93, .	3.2	166
12	Kapitza conductance of siliconâ€“amorphous polyethylene interfaces by molecular dynamics simulations. Physical Review B, 2009, 79, .	3.2	165
13	Thermal conductivity of silicene from first-principles. Applied Physics Letters, 2014, 104, .	3.3	155
14	Orbitally driven low thermal conductivity of monolayer gallium nitride (GaN) with planar honeycomb structure: a comparative study. Nanoscale, 2017, 9, 4295-4309.	5.6	155
15	On the Mechanism of Hydrophilicity of Graphene. Nano Letters, 2016, 16, 4447-4453.	9.1	148
16	Generative adversarial networks (GAN) based efficient sampling of chemical composition space for inverse design of inorganic materials. Npj Computational Materials, 2020, 6, .	8.7	117
17	Resonant bonding driven giant phonon anharmonicity and low thermal conductivity of phosphorene. Physical Review B, 2016, 94, .	3.2	114
18	Interfacial thermal conductance between silicon and a vertical carbon nanotube. Journal of Applied Physics, 2008, 104, .	2.5	103

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19	Anomalously temperature-dependent thermal conductivity of monolayer GaN with large deviations from the traditional <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mn>1</mml:mn><mml:mo>/</mml:mo><mml:mi>T</mml:mi></mml:ma law. Physical Review B, 2017, 95, .	3.2	101
20	Sub-amorphous Thermal Conductivity in Ultrathin Crystalline Silicon Nanotubes. Nano Letters, 2015, 15, 2605-2611.	9.1	94
21	Thermal conductivity reduction in core-shell nanowires. Physical Review B, 2011, 84, .	3.2	92
22	Thermal rectification at silicon-amorphous polyethylene interface. Applied Physics Letters, 2008, 92, 211908.	3.3	88
23	Bilateral substrate effect on the thermal conductivity of two-dimensional silicon. Nanoscale, 2015, 7, 6014-6022.	5.6	80
24	Large improvement of thermal transport and mechanical performance of polyvinyl alcohol composites based on interface enhanced by SiO2 nanoparticle-modified-hexagonal boron nitride. Composites Science and Technology, 2019, 169, 167-175.	7.8	80
25	Phonon interference at self-assembled monolayer interfaces: Molecular dynamics simulations. Physical Review B, 2010, 81, .	3.2	79
26	Water Nanoconfinement Induced Thermal Enhancement at Hydrophilic Quartz Interfaces. Nano Letters, 2010, 10, 279-285.	9.1	76
27	Full quantification of frequency-dependent interfacial thermal conductance contributed by two- and three-phonon scattering processes from nonequilibrium molecular dynamics simulations. Physical Review B, 2017, 95, .	3.2	75
28	Molecular dynamics simulation of interfacial thermal conductance between silicon and amorphous polyethylene. Applied Physics Letters, 2007, 91, .	3.3	71
29	Enhanced thermal conductivity of free-standing 3D hierarchical carbon nanotube-graphene hybrid paper. Composites Part A: Applied Science and Manufacturing, 2017, 102, 1-8.	7.6	70
30	Competing mechanism driving diverse pressure dependence of thermal conductivity of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>X</mml:mi><mml:mtext>Te</mml:mtext></mml:math><mml:math		

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37	An excellent candidate for largely reducing interfacial thermal resistance: a nano-confined mass graded interface. Nanoscale, 2016, 8, 1994-2002.	5.6	59
38	Thermal transport properties of GaN with biaxial strain and electron-phonon coupling. Journal of Applied Physics, 2020, 127, .	2.5	59
39	Graphene mediated thermal resistance reduction at strongly coupled interfaces. International Journal of Heat and Mass Transfer, 2013, 62, 205-213.	4.8	57
40	Nonmonotonic Diameter Dependence of Thermal Conductivity of Extremely Thin Si Nanowires: Competition between Hydrodynamic Phonon Flow and Boundary Scattering. Nano Letters, 2017, 17, 1269-1276.	9.1	56
41	Surface Functionalization Mechanisms of Enhancing Heat Transfer at Solid-Liquid Interfaces. Journal of Heat Transfer, 2011, 133, .	2.1	55
42	Low thermal conductivity of monolayer ZnO and its anomalous temperature dependence. Physical Chemistry Chemical Physics, 2017, 19, 12882-12889.	2.8	55
43	Lone-pair electrons induced anomalous enhancement of thermal transport in strained planar two-dimensional materials. Nano Energy, 2018, 50, 425-430.	16.0	55
44	Nontrivial contribution of FrÃ¶hlich electron-phonon interaction to lattice thermal conductivity of wurtzite GaN. Applied Physics Letters, 2016, 109, .	3.3	53
45	Insight into the collective vibrational modes driving ultralow thermal conductivity of perovskite solar cells. Physical Review B, 2016, 94, .	3.2	52
46	Molecular Origin of Electric Double-Layer Capacitance at Multilayer Graphene Edges. Journal of Physical Chemistry Letters, 2017, 8, 153-160.	4.6	52
47	Thermal rectification at silicon/horizontally aligned carbon nanotube interfaces. Journal of Applied Physics, 2013, 113, 194307.	2.5	51
48	Thermal transport and thermoelectric properties of beta-graphyne nanostructures. Nanotechnology, 2014, 25, 245401.	2.6	51
49	Accelerating evaluation of converged lattice thermal conductivity. Npj Computational Materials, 2018, 4, .	8.7	50
50	A Low-Frequency Wave Motion Mechanism Enables Efficient Energy Transport in Carbon Nanotubes at High Heat Fluxes. Nano Letters, 2012, 12, 3410-3416.	9.1	47
51	Origin of anisotropic negative Poisson's ratio in graphene. Nanoscale, 2018, 10, 10365-10370.	5.6	43
52	Thermal transport in novel carbon allotropes with <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>s</mml:mi><mml:msup><mml:mi>p</mml:mi><mml:mn> or <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>s</mml:mi><mml:msup><mml:mi>p</mml:mi><mml:mn> hybridization: An ab initio study. Physical Review B, 2017, 95, .	3.2	42
53	Anomalous pressure effect on the thermal conductivity of ZnO, GaN, and AlN from first-principles calculations. Physical Review B, 2018, 98, .	3.2	42
54	Enhancement of interfacial thermal transport by carbon nanotube-graphene junction. Journal of Applied Physics, 2014, 115, .	2.5	40

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55	Mechanics of nanoscale wrinkling of graphene on a non-developable surface. Carbon, 2015, 84, 263-271.	10.3	40
56	Thermal transport crossover from crystalline to partial-crystalline partial-liquid state. Nature Communications, 2018, 9, 4712.	12.8	39
57	Lone-Pair Electrons Do Not Necessarily Lead to Low Lattice Thermal Conductivity: An Exception of Two-Dimensional Penta-CN₂. Journal of Physical Chemistry Letters, 2018, 9, 2474-2483.	4.6	38
58	Exploring T-carbon for energy applications. Nanoscale, 2019, 11, 5798-5806.	5.6	38
59	Highâ€Throughput Discovery of Novel Cubic Crystal Materials Using Deep Generative Neural Networks. Advanced Science, 2021, 8, e2100566.	11.2	38
60	Quantitatively analyzing phonon spectral contribution of thermal conductivity based on nonequilibrium molecular dynamics simulations. II. From time Fourier transform. Physical Review B, 2015, 92, .	3.2	37
61	Thermodynamic and Transport Properties of LiF and FLiBe Molten Salts with Deep Learning Potentials. ACS Applied Materials & Interfaces, 2021, 13, 55367-55379.	8.0	37
62	Anisotropic thermal transport in Weyl semimetal TaAs: a first principles calculation. Physical Chemistry Chemical Physics, 2016, 18, 16709-16714.	2.8	36
63	Thermal Transport in Phosphorene. Small, 2018, 14, e1702465.	10.0	36
64	Diameter Dependence of Lattice Thermal Conductivity of Single-Walled Carbon Nanotubes: Study from Ab Initio. Scientific Reports, 2015, 5, 15440.	3.3	35
65	Probing phononâ€“surface interaction by wave-packet simulation: Effect of roughness and morphology. Journal of Applied Physics, 2017, 122, .	2.5	35
66	Strong anharmonic phonon scattering induced giant reduction of thermal conductivity in PbTe nanotwin boundary. Physical Review B, 2018, 97, .	3.2	34
67	On the diversity in the thermal transport properties of graphene: A first-principles-benchmark study testing different exchange-correlation functionals. Computational Materials Science, 2018, 151, 153-159.	3.0	34
68	Large â€œnear junctionâ€•thermal resistance reduction in electronics by interface nanoengineering. International Journal of Heat and Mass Transfer, 2011, 54, 5183-5183.	4.8	32
69	Tutorial: Determination of thermal boundary resistance by molecular dynamics simulations. Journal of Applied Physics, 2018, 123, .	2.5	32
70	Lattice Thermal Conductivity Prediction Using Symbolic Regression and Machine Learning. Journal of Physical Chemistry A, 2021, 125, 435-450.	2.5	32
71	Decouple electronic and phononic transport in nanotwinned structures: a new strategy for enhancing the figure-of-merit of thermoelectrics. Nanoscale, 2017, 9, 9987-9996.	5.6	31
72	Giant effect of spinâ€“lattice coupling on the thermal transport in two-dimensional ferromagnetic CrI₃. Journal of Materials Chemistry C, 2020, 8, 3520-3526.	5.5	31

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73	Thermal energy exchange between carbon nanotube and air. Applied Physics Letters, 2007, 90, 231905.	3.3	29
74	First-principles study of thermal transport in nitrogenated holey graphene. Nanotechnology, 2017, 28, 045709.	2.6	29
75	Temperature-Induced Large Broadening and Blue Shift in the Electronic Band Structure and Optical Absorption of Methylammonium Lead Iodide Perovskite. Journal of Physical Chemistry Letters, 2017, 8, 3720-3725.	4.6	29
76	Strong phonon localization in PbTe with dislocations and large deviation to Matthiessenâ€™s rule. Npj Computational Materials, 2019, 5, .	8.7	29
77	Thermal conductivity of ordered-disordered material: a case study of superionic Ag₂Te. Nanotechnology, 2015, 26, 025702.	2.6	27
78	On the origin of abnormal phonon transport of graphyne. International Journal of Heat and Mass Transfer, 2015, 85, 880-889.	4.8	27
79	Robustly Engineering Thermal Conductivity of Bilayer Graphene by Interlayer Bonding. Scientific Reports, 2016, 6, 22011.	3.3	27
80	The typical manners of dynamic crack propagation along the metal/ceramics interfaces: A molecular dynamics study. Computational Materials Science, 2016, 112, 27-33.	3.0	26
81	Metric for strong intrinsic fourth-order phonon anharmonicity. Physical Review B, 2017, 95, .	3.2	26
82	The intrinsic thermal transport properties of the biphenylene network and the influence of hydrogenation: a first-principles study. Journal of Materials Chemistry C, 2021, 9, 16945-16951.	5.5	26
83	Thermal conductivity of hybrid graphene/silicon heterostructures. Journal of Applied Physics, 2013, 114, .	2.5	25
84	Mechanical behaviors of nanocrystalline Cu/SiC composites: An atomistic investigation. Computational Materials Science, 2017, 129, 129-136.	3.0	25
85	Four-Phonon Scattering Effect and Two-Channel Thermal Transport in Two-Dimensional Paraelectric SnSe. ACS Applied Materials & Interfaces, 2022, 14, 11493-11499.	8.0	25
86	Schemes for and Mechanisms of Reduction in Thermal Conductivity in Nanostructured Thermoelectrics. Journal of Heat Transfer, 2012, 134, .	2.1	24
87	The unexpected non-monotonic inter-layer bonding dependence of the thermal conductivity of bilayered boron nitride. Nanoscale, 2015, 7, 7143-7150.	5.6	24
88	Unusual Thermal Boundary Resistance in Halide Perovskites: A Way To Tune Ultralow Thermal Conductivity for Thermoelectrics. ACS Applied Materials & Interfaces, 2019, 11, 47507-47515.	8.0	24
89	Recrystallization of picosecond laser-melted ZnO nanoparticles in a liquid: A molecular dynamics study. Journal of Chemical Physics, 2010, 132, 164504.	3.0	23
90	Thermal boundary conductance enhancement using experimentally achievable nanostructured interfaces â€“ analytical study combined with molecular dynamics simulation. Physical Chemistry Chemical Physics, 2016, 18, 16794-16801.	2.8	23

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91	Ultrahigh thermal conductivity of carbon allotropes with correlations with the scaled Pugh ratio. Journal of Materials Chemistry A, 2019, 7, 6259-6266.	10.3	23
92	Unexpected anisotropy of (14,14,14)-Graphyne: A comprehensive study on the thermal transport properties of graphyne based nanomaterials. Carbon, 2019, 143, 189-199.	10.3	23
93	Predicting Elastic Properties of Materials from Electronic Charge Density Using 3D Deep Convolutional Neural Networks. Journal of Physical Chemistry C, 2020, 124, 17262-17273.	3.1	23
94	Intrinsically low lattice thermal conductivity of monolayer hexagonal aluminum nitride (h-AlN) from first-principles: A comparative study with graphene. International Journal of Thermal Sciences, 2021, 162, 106772.	4.9	23
95	High-Throughput Computation of New Carbon Allotropes with Diverse Hybridization and Ultrahigh Hardness. Crystals, 2021, 11, 783.	2.2	23
96	Unusual strain response of thermal transport in dimerized three-dimensional graphene. Nanoscale, 2018, 10, 5229-5238.	5.6	22
97	The exceptionally high thermal conductivity after â€˜alloyingâ€™ two-dimensional gallium nitride (GaN) and aluminum nitride (AlN). Nanotechnology, 2021, 32, 135401.	2.6	22
98	Metavalent bonding induced abnormal phonon transport in diamondlike structures: Beyond conventional theory. Physical Review B, 2021, 103, .	3.2	22
99	Two-dimensional magnetic metalâ€“organic frameworks with the Shastry-Sutherland lattice. Chemical Science, 2019, 10, 10381-10387.	7.4	21
100	High-throughput computation of novel ternary Bâ€“Câ€“N structures and carbon allotropes with electronic-level insights into superhard materials from machine learning. Journal of Materials Chemistry A, 2021, 9, 27596-27614.	10.3	21
101	Strong Surface Orientation Dependent Thermal Transport in Si Nanowires. Scientific Reports, 2016, 6, 24903.	3.3	20
102	Phonon transport in the ground state of two-dimensional silicon and germanium. RSC Advances, 2016, 6, 69956-69965.	3.6	20
103	Extremely Low Thermal Conductivity of Polycrystalline Silicene. Journal of Physical Chemistry C, 2018, 122, 9220-9228.	3.1	20
104	Spatial density neural network force fields with first-principles level accuracy and application to thermal transport. Physical Review B, 2020, 102, .	3.2	20
105	Strain-modulated electronic and thermal transport properties of two-dimensional O-silica. Nanotechnology, 2016, 27, 265706.	2.6	18
106	Giant reduction in thermal conductivity of extended type-I silicon clathrates and prominent thermal effect of 6d guest Wyckoff positions. Journal of Materials Chemistry C, 2017, 5, 10578-10588.	5.5	18
107	Machine Learning based prediction of noncentrosymmetric crystal materials. Computational Materials Science, 2020, 183, 109792.	3.0	18
108	Molecular/cluster statistical thermodynamics methods to simulate quasi-static deformations at finite temperature. International Journal of Solids and Structures, 2008, 45, 3918-3933.	2.7	17

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109	Methodology for determining the electronic thermal conductivity of metals via direct nonequilibriumab initiomolecular dynamics. Physical Review B, 2016, 94, .	3.2	17
110	First-principles study on lattice thermal conductivity of thermoelectrics HgTe in different phases. Journal of Applied Physics, 2015, 117, .	2.5	16
111	Surface Chemical Tuning of Phonon and Electron Transport in Free-Standing Silicon Nanowire Arrays. Nano Letters, 2016, 16, 6364-6370.	9.1	16
112	Enormous suppression of phonon transport in silicon nanowires with five-fold twin boundary. Journal of Materials Chemistry A, 2018, 6, 18533-18542.	10.3	16
113	An LCâ€“MS/MS method for simultaneous determination of nine steroidal saponins from Paris polyphylla var. in rat plasma and its application to pharmacokinetic study. Journal of Pharmaceutical and Biomedical Analysis, 2017, 145, 675-681.	2.8	15
114	Bond saturation significantly enhances thermal energy transport in two-dimensional pentagonal materials. Nano Energy, 2018, 45, 1-9.	16.0	15
115	Electric field tuned anisotropic to isotropic thermal transport transition in monolayer borophene without altering its atomic structure. Nanoscale, 2020, 12, 19178-19190.	5.6	15
116	Strong electron-phonon coupling induced anomalous phonon transport in ultrahigh temperature ceramics ZrB2 and TiB2. International Journal of Heat and Mass Transfer, 2020, 152, 119481.	4.8	15
117	The role of phononâ€“phonon and electronâ€“phonon scattering in thermal transport in PdCoO₂. Physical Chemistry Chemical Physics, 2017, 19, 21714-21721.	2.8	14
118	Development of a validated UPLCâ€“MS/MS method for determination of humantenmine in rat plasma and its application in pharmacokinetics and bioavailability studies. Biomedical Chromatography, 2017, 31, e4017.	1.7	13
119	Enhanced thermoelectric properties of the AGNRâ€“GYNR heterojunctions. Physics Letters, Section A: General, Atomic and Solid State Physics, 2017, 381, 3766-3772.	2.1	13
120	Why thermal conductivity of CaO is lower than that of CaS: a study from the perspective of phonon splitting of optical mode. Nanotechnology, 2021, 32, 025709.	2.6	13
121	First-principles and molecular dynamics study of thermoelectric transport properties of N-type silicon-based superlattice-nanocrystalline heterostructures. Journal of Applied Physics, 2017, 122, 085105.	2.5	12
122	Unprecedented mechanical response of the lattice thermal conductivity of auxetic carbon crystals. Carbon, 2017, 122, 374-380.	10.3	12
123	A C20 fullerene-based sheet with ultrahigh thermal conductivity. Nanoscale, 2018, 10, 6099-6104.	5.6	12
124	Unconventional thermal transport enhancement with large atom mass: a comparative study of 2D transition dichalcogenides. 2D Materials, 2018, 5, 015022.	4.4	12
125	Electronâ€“phonon interaction and superconductivity in the high-pressure cI16 phase of lithium from first principles. Physical Chemistry Chemical Physics, 2018, 20, 27125-27130.	2.8	12
126	Two-Channel Thermal Transport in Orderedâ€“Disordered Superionic Ag₂Te and Its Traditionally Contradictory Enhancement by Nanotwin Boundary. Journal of Physical Chemistry Letters, 2018, 9, 5704-5709.	4.6	12

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127	BaWO₂F₄: a mixed anion X-ray scintillator with excellent photoluminescence quantum efficiency. Dalton Transactions, 2020, 49, 10734-10739.	3.3	12
128	Sustainable design rating system comparison using a life-cycle methodology. Building and Environment, 2017, 126, 410-421.	6.9	11
129	Unravelling the progressive role of rattlers in thermoelectric clathrate and strategies for performance improvement: Concurrently enhancing electronic transport and blocking phononic transport. Applied Physics Letters, 2017, 111, .	3.3	11
130	Methodology Perspective of Computing Thermal Transport in Low-Dimensional Materials and Nanostructures: The Old and the New. ACS Omega, 2018, 3, 3278-3284.	3.5	11
131	Molecular dynamics simulations of the effect of dislocations on the thermal conductivity of iron. Journal of Applied Physics, 2020, 127, 045106.	2.5	11
132	Fluorideâ€Based Anion Doping: A New Strategy for Improving the Performance of Protonic Ceramic Conductors of the Form BaZrO₃. ChemElectroChem, 2020, 7, 2242-2247.	3.4	11
133	Perspective on multi-scale simulation of thermal transport in solids and interfaces. Physical Chemistry Chemical Physics, 2021, 23, 1785-1801.	2.8	11
134	Phonon transport anomaly in metavalent bonded materials: contradictory to the conventional theory. Journal of Materials Science, 2021, 56, 18534-18549.	3.7	11
135	Interfacial mixing during annealing of zinc oxide nanoparticle junctions. Applied Physics Letters, 2011, 98, .	3.3	9
136	Thermal conductivity of oxidized gamma-graphyne. RSC Advances, 2015, 5, 65221-65226.	3.6	9
137	Dependence of phonon transport properties with stacking thickness in layered ZnO. Journal Physics D: Applied Physics, 2018, 51, 315303.	2.8	9
138	Improvement of Thermoelectricity Through Magnetic Interactions in Layered Cr₂Ge₂Te₆. Physica Status Solidi - Rapid Research Letters, 2018, 12, 1800172.	2.4	9
139	Probing the phonon mean free paths in dislocation core by molecular dynamics simulation. Journal of Applied Physics, 2021, 129, .	2.5	9
140	Air flow through carbon nanotube arrays. Applied Physics Letters, 2007, 91, 131905.	3.3	8
141	Surface segregation of bimetallic alloys in nanoscale confinement. Applied Physics Letters, 2010, 97, .	3.3	8
142	Boundary scattering effect on the thermal conductivity of nanowires. Semiconductor Science and Technology, 2016, 31, 074004.	2.0	8
143	Accurate quantification of PGE 2 in the polyposis in rat colon (Pirc) model by surrogate analyte-based UPLCâ€“MS/MS. Journal of Pharmaceutical and Biomedical Analysis, 2018, 148, 42-50.	2.8	8
144	Decoupling thermal and electrical transport in Î±-MgAgSb with synergic pressure and doping strategy. Journal of Applied Physics, 2019, 125, .	2.5	8

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145	First Principles Investigation of Anomalous Pressure-Dependent Thermal Conductivity of Chalcopyrites. Materials, 2019, 12, 3491.	2.9	8
146	Electronic charge density as a fast approach for predicting Li-ion migration pathways in superionic conductors with first-principles level precision. Computational Materials Science, 2021, 192, 110380.	3.0	8
147	Efficiently searching extreme mechanical properties via boundless objective-free exploration and minimal first-principles calculations. Npj Computational Materials, 2022, 8, .	8.7	8
148	Multi-scale analysis of AFM tip and surface interactions. Chemical Engineering Science, 2007, 62, 3589-3594.	3.8	7
149	Ground state of bilayer hÎ±-silica: mechanical and electronic properties. Nanotechnology, 2015, 26, 505702.	2.6	7
150	Hyperelastic material modeling of graphene based on density functional calculations. Proceedings in Applied Mathematics and Mechanics, 2018, 18, e201800419.	0.2	7
151	Thermoelectric properties of four typical silicon allotropes. Modelling and Simulation in Materials Science and Engineering, 2018, 26, 085006.	2.0	7
152	Strong electronâ€“phonon interaction retarding phonon transport in superconducting hydrogen sulfide at high pressures. Physical Chemistry Chemical Physics, 2018, 20, 24222-24226.	2.8	7
153	Phonon scattering in the complex strain field of a dislocation in PbTe. Journal of Materials Chemistry C, 2021, 9, 8506-8514.	5.5	7
154	Doping Induced Abnormal Contraction and Significant Reduction of Lattice Thermal Conductivity of Open Framework Si24. ES Energy & Environments, 2018, , .	1.1	7
155	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
156	Bidirectional effect of magnetic field on electronic thermal transport of metals from all-electron first-principles calculations. Physical Review B, 2016, 94, .	3.2	6
157	Spin-dependent Seebeck effects in a graphene superlatticepâ€“njunction with different shapes. Journal of Physics Condensed Matter, 2017, 29, 405303.	1.8	6
158	Thermal transport properties of monolayer phosphorene: a mini-review of theoretical studies. Frontiers in Energy, 2018, 12, 87-96.	2.3	6
159	Insight of the thermal conductivity of Ïµ-iron at Earthâ€™s core conditions from the newly developed direct ab initio methodology. Journal of Applied Physics, 2019, 125, .	2.5	5
160	Strong laser polarization control of coherent phonon excitation in van der Waals material Fe3GeTe2. Npj 2D Materials and Applications, 2022, 6, .	7.9	5
161	Electrically-driven robust tuning of lattice thermal conductivity. Physical Chemistry Chemical Physics, 2022, 24, 17479-17484.	2.8	5
162	Exploration of exciton behavior in atomically thin WS2 layers by ionic gating. Applied Physics Letters, 2018, 113, .	3.3	4

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163	A nonlinear hyperelasticity model for single layer blue phosphorus based on ab initio calculations. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2019, 475, 20190149.	2.1	4
164	Hydrothermal syntheses and crystal structures of molybdenum tellurites. Journal of Solid State Chemistry, 2020, 287, 121317.	2.9	4
165	Enhanced Two-Photon Absorption in Two Triphenylamine-Based All-Organic Compounds. Journal of Physical Chemistry A, 2021, 125, 1870-1879.	2.5	4
166	Ab Initio Energetic Barriers of Gas Permeation across Nanoporous Graphene. ACS Applied Materials & Interfaces, 2021, 13, 39701-39710.	8.0	4
167	Cluster Statistical Thermodynamics (CST) â€" To Efficiently Calculate Quasi-Static Deformation at Finite Temperature Based on Molecular Potential. , 2007, , 163-170.		4
168	Giant Manipulation of Phonon Hydrodynamics in Ferroelectric Bilayer Boron Nitride at Room Temperature and Beyond. ACS Applied Energy Materials, 2022, 5, 8781-8790.	5.1	4
169	Diverse Thermal Transport Properties of Two-Dimensional Materials: A Comparative Review. , 0, , .		2
170	Tailoring thermal conductivity of AlN films by periodically aligned surface nano-grooves. Applied Physics Letters, 2016, 109, 133107.	3.3	2
171	Analytical study on the size effect of phonon spectral energy density resolution. Computational Materials Science, 2017, 132, 6-9.	3.0	2
172	The lattice thermal conductivity in monolayers group-VA: from elements to binary compounds. Materials Research Express, 2021, 8, 075007.	1.6	2
173	Nonlocality Effect in Atomic Force Microscopy Measurement and Its Reduction by an Approaching Method. Journal of Engineering Materials and Technology, Transactions of the ASME, 2005, 127, 444-450.	1.4	1
174	Uniform Strain-Dependent Thermal Conductivity of Pentagonal and Hexagonal Silicene. Frontiers in Materials, 2021, 8, .	2.4	1
175	Large scale dataset of real space electronic charge density of cubic inorganic materials from density functional theory (DFT) calculations. Scientific Data, 2022, 9, 59.	5.3	1
176	Significant Enhancement of Two-Photon Excited Fluorescence in Water-Soluble Triphenylamine-Based All-Organic Compounds. Journal of Physical Chemistry B, 2022, 126, 5513-5522.	2.6	1
177	Equivalency and Locality in Nano-scale Measurement. International Journal of Nonlinear Sciences and Numerical Simulation, 2005, 6, .	1.0	0
178	Molecular Dynamics Simulation of Thermal Conductivity of Diamondoid Crystals. Materials Research Society Symposia Proceedings, 2007, 1022, 1.	0.1	0
179	Surface Functionalization Mechanisms of Enhancing Heat Transfer at Solid-Liquid Interfaces. , 2010, , .		0
180	Enhancement of Interfacial Thermal Transport by Carbon Nanotube-Graphene Junction. , 2013, , .		0

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181	On the development of continuum material models for 2D materials from Density Functional Theory data. Proceedings in Applied Mathematics and Mechanics, 2019, 19, e201900486.	0.2	0
182	Activated Lone-Pair Electrons Lead to Low Lattice Thermal Conductivity: A Case Study of Boron Arsenide. SSRN Electronic Journal, 0, , .	0.4	0
183	Two-dimensional silicon. Series in Materials Science and Engineering, 2017, , 43-76.	0.1	0
184	Si nanowires for evolutionary nanotechnology. Series in Materials Science and Engineering, 2017, , 515-536.	0.1	0
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