Ming Hu

List of Publications by Citations

171 papers	5,426 citations	40 h-index	67 g-index
189 ext. papers	6,463 ext. citations	5.2 avg, IF	6.37 L-index

#	Paper	IF	Citations
171	Anisotropic intrinsic lattice thermal conductivity of phosphorene from first principles. *Physical Chemistry Chemical Physics*, **2015**, 17, 4854-8	3.6	296
170	Significant reduction of thermal conductivity in Si/Ge core-shell nanowires. *Nano Letters*, **2011**, 11, 618-23	11.5	184
169	Thermal conductivity of silicene calculated using an optimized Stillinger-Weber potential. *Physical Review B*, **2014**, 89,	3.3	173
168	Diverse anisotropy of phonon transport in two-dimensional group IV-VI compounds: A comparative study. *Nanoscale*, **2016**, 8, 11306-19	7.7	170
167	Si/Ge superlattice nanowires with ultralow thermal conductivity. *Nano Letters*, **2012**, 12, 5487-94	11.5	168
166	Anomalous thermal response of silicene to uniaxial stretching. *Physical Review B*, **2013**, 87,	3.3	151
165	Kapitza conductance of silicon□amorphous polyethylene interfaces by molecular dynamics simulations. *Physical Review B*, **2009**, 79,	3.3	147
164	Hot-pressing induced alignment of boron nitride in polyurethane for composite films with thermal conductivity over 50 Wm□1 K□1. *Composites Science and Technology*, **2018**, 160, 199-207	8.6	144
163	A facile method to prepare flexible boron nitride/poly(vinyl alcohol) composites with enhanced thermal conductivity. *Composites Science and Technology*, **2017**, 149, 41-47	8.6	138
162	Large tunability of lattice thermal conductivity of monolayer silicene via mechanical strain. *Physical Review B*, **2016**, 93,	3.3	132
161	Disparate Strain Dependent Thermal Conductivity of Two-dimensional Penta-Structures. *Nano Letters*, **2016**, 16, 3831-42	11.5	132
160	Thermal conductivity of silicene from first-principles. *Applied Physics Letters*, **2014**, 104, 131906	3.4	123
159	On the Mechanism of Hydrophilicity of Graphene. *Nano Letters*, **2016**, 16, 4447-53	11.5	102
158	Orbitally driven low thermal conductivity of monolayer gallium nitride (GaN) with planar honeycomb structure: a comparative study. *Nanoscale*, **2017**, 9, 4295-4309	7.7	101
157	Interfacial thermal conductance between silicon and a vertical carbon nanotube. *Journal of Applied Physics*, **2008**, 104, 083503	2.5	89
156	Thermal conductivity reduction in core-shell nanowires. *Physical Review B*, **2011**, 84,	3.3	87
155	Thermal rectification at silicon-amorphous polyethylene interface. *Applied Physics Letters*, **2008**, 92, 211908	3.4	85

154	Sub-amorphous thermal conductivity in ultrathin crystalline silicon nanotubes. *Nano Letters*, **2015**, 15, 2605-11	11.5	83
153	Resonant bonding driven giant phonon anharmonicity and low thermal conductivity of phosphorene. *Physical Review B*, **2016**, 94,	3.3	79
152	Phonon interference at self-assembled monolayer interfaces: Molecular dynamics simulations. *Physical Review B*, **2010**, 81,	3.3	78
151	Evaluating explorative prediction power of machine learning algorithms for materials discovery using k-fold forward cross-validation. *Computational Materials Science*, **2020**, 171, 109203	3.2	77
150	Bilateral substrate effect on the thermal conductivity of two-dimensional silicon. *Nanoscale*, **2015**, 7, 6014-22	7.7	71
149	Anomalously temperature-dependent thermal conductivity of monolayer GaN with large deviations from the traditional 1/T law. *Physical Review B*, **2017**, 95,	3.3	71
148	Molecular dynamics simulation of interfacial thermal conductance between silicon and amorphous polyethylene. *Applied Physics Letters*, **2007**, 91, 241910	3.4	62
147	Water nanoconfinement induced thermal enhancement at hydrophilic quartz interfaces. *Nano Letters*, **2010**, 10, 279-85	11.5	60
146	Low thermal conductivity of graphyne nanotubes from molecular dynamics study. *Physical Review B* , **2015**, 91,	3.3	57
145	Thermal rectification at water/functionalized silica interfaces. *Applied Physics Letters*, **2009**, 95, 151903	3.4	57
144	Enhanced thermal conductivity of free-standing 3D hierarchical carbon nanotube-graphene hybrid paper. *Composites Part A: Applied Science and Manufacturing*, **2017**, 102, 1-8	8.4	53
143	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	8.6	52
142	Competing mechanism driving diverse pressure dependence of thermal conductivity of XTe (X=Hg,Cd, and Zn). *Physical Review B*, **2015**, 92,	3.3	51
141	Quantitatively analyzing phonon spectral contribution of thermal conductivity based on nonequilibrium molecular dynamics simulations. I. From space Fourier transform. *Physical Review B*, **2015**, 92,	3.3	49
140	Surface Functionalization Mechanisms of Enhancing Heat Transfer at Solid-Liquid Interfaces. *Journal of Heat Transfer*, **2011**, 133,	1.8	47
139	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	11.5	45
138	Thermal transport and thermoelectric properties of beta-graphyne nanostructures. *Nanotechnology*, **2014**, 25, 245401	3.4	45
137	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,	3.3	44

136	An excellent candidate for largely reducing interfacial thermal resistance: a nano-confined mass graded interface. *Nanoscale*, **2016**, 8, 1994-2002	7.7	44
135	Record Low Thermal Conductivity of Polycrystalline Si Nanowire: Breaking the Casimir Limit by Severe Suppression of Propagons. *Nano Letters*, **2016**, 16, 6178-6187	11.5	44
134	Graphene mediated thermal resistance reduction at strongly coupled interfaces. *International Journal of Heat and Mass Transfer*, **2013**, 62, 205-213	4.9	42
133	A low-frequency wave motion mechanism enables efficient energy transport in carbon nanotubes at high heat fluxes. *Nano Letters*, **2012**, 12, 3410-6	11.5	42
132	Insight into the collective vibrational modes driving ultralow thermal conductivity of perovskite solar cells. *Physical Review B*, **2016**, 94,	3.3	41
131	Thermal rectification at silicon/horizontally aligned carbon nanotube interfaces. *Journal of Applied Physics*, **2013**, 113, 194307	2.5	40
130	External electric field driving the ultra-low thermal conductivity of silicene. *Nanoscale*, **2017**, 9, 7227-7234	7.7	39
129	Generative adversarial networks (GAN) based efficient sampling of chemical composition space for inverse design of inorganic materials. *Npj Computational Materials*, **2020**, 6,	10.9	39
128	Molecular Origin of Electric Double-Layer Capacitance at Multilayer Graphene Edges. *Journal of Physical Chemistry Letters*, **2017**, 8, 153-160	6.4	38
127	Low thermal conductivity of monolayer ZnO and its anomalous temperature dependence. *Physical Chemistry Chemical Physics*, **2017**, 19, 12882-12889	3.6	37
126	Enhancement of interfacial thermal transport by carbon nanotube-graphene junction. *Journal of Applied Physics*, **2014**, 115, 053524	2.5	36
125	Nontrivial contribution of Fröhlich electron-phonon interaction to lattice thermal conductivity of wurtzite GaN. *Applied Physics Letters*, **2016**, 109, 242103	3.4	34
124	Mechanics of nanoscale wrinkling of graphene on a non-developable surface. *Carbon*, **2015**, 84, 263-271	10.4	33
123	Thermal transport in novel carbon allotropes with sp2 or sp3 hybridization: An ab initio study. *Physical Review B*, **2017**, 95,	3.3	32
122	First-principles study of electronic, optical and thermal transport properties of group III–VI monolayer MX (M = Ga, In; X = S, Se). *Journal of Applied Physics*, **2019**, 125, 245104	2.5	32
121	Lone-pair electrons induced anomalous enhancement of thermal transport in strained planar two-dimensional materials. *Nano Energy*, **2018**, 50, 425-430	17.1	32
120	Thermal transport properties of GaN with biaxial strain and electron-phonon coupling. *Journal of Applied Physics*, **2020**, 127, 035102	2.5	29
119	Exploring T-carbon for energy applications. *Nanoscale*, **2019**, 11, 5798-5806	7.7	28

118	Quantitatively analyzing phonon spectral contribution of thermal conductivity based on nonequilibrium molecular dynamics simulations. II. From time Fourier transform. *Physical Review B*, **2015**, 92,	3.3	28
117	Diameter Dependence of Lattice Thermal Conductivity of Single-Walled Carbon Nanotubes: Study from Ab Initio. *Scientific Reports*, **2015**, 5, 15440	4.9	27
116	Thermal energy exchange between carbon nanotube and air. *Applied Physics Letters*, **2007**, 90, 231905	3.4	27
115	Accelerating evaluation of converged lattice thermal conductivity. *Npj Computational Materials*, **2018**, 4,	10.9	26
114	Anisotropic thermal transport in Weyl semimetal TaAs: a first principles calculation. *Physical Chemistry Chemical Physics*, **2016**, 18, 16709-14	3.6	26
113	Robustly Engineering Thermal Conductivity of Bilayer Graphene by Interlayer Bonding. *Scientific Reports*, **2016**, 6, 22011	4.9	25
112	Thermal Transport in Phosphorene. *Small*, **2018**, 14, e1702465	11	24
111	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	3.2	24
110	First-principles study of thermal transport in nitrogenated holey graphene. *Nanotechnology*, **2017**, 28, 045709	3.4	23
109	Strong anharmonic phonon scattering induced giant reduction of thermal conductivity in PbTe nanotwin boundary. *Physical Review B*, **2018**, 97,	3.3	23
108	The typical manners of dynamic crack propagation along the metal/ceramics interfaces: A molecular dynamics study. *Computational Materials Science*, **2016**, 112, 27-33	3.2	23
107	Probing phonon–surface interaction by wave-packet simulation: Effect of roughness and morphology. *Journal of Applied Physics*, **2017**, 122, 155104	2.5	23
106	Decouple electronic and phononic transport in nanotwinned structures: a new strategy for enhancing the figure-of-merit of thermoelectrics. *Nanoscale*, **2017**, 9, 9987-9996	7.7	23
105	Thermal conductivity of ordered-disordered material: a case study of superionic Ag2Te. *Nanotechnology*, **2015**, 26, 025702	3.4	23
104	Schemes for and Mechanisms of Reduction in Thermal Conductivity in Nanostructured Thermoelectrics. *Journal of Heat Transfer*, **2012**, 134,	1.8	23
103	Thermal transport crossover from crystalline to partial-crystalline partial-liquid state. *Nature Communications*, **2018**, 9, 4712	17.4	23
102	Origin of anisotropic negative Poisson's ratio in graphene. *Nanoscale*, **2018**, 10, 10365-10370	7.7	22
101	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	6.4	22

100	Tutorial: Determination of thermal boundary resistance by molecular dynamics simulations. *Journal of Applied Physics*, **2018**, 123, 191101	2.5	22
99	The unexpected non-monotonic inter-layer bonding dependence of the thermal conductivity of bilayered boron nitride. *Nanoscale*, **2015**, 7, 7143-50	7.7	21
98	On the origin of abnormal phonon transport of graphyne. *International Journal of Heat and Mass Transfer*, **2015**, 85, 880-889	4.9	21
97	Recrystallization of picosecond laser-melted ZnO nanoparticles in a liquid: a molecular dynamics study. *Journal of Chemical Physics*, **2010**, 132, 164504	3.9	20
96	Strong phonon localization in PbTe with dislocations and large deviation to Matthiessen□s rule. *Npj Computational Materials*, **2019**, 5,	10.9	19
95	Metric for strong intrinsic fourth-order phonon anharmonicity. *Physical Review B*, **2017**, 95,	3.3	19
94	Large □ear junction□thermal resistance reduction in electronics by interface nanoengineering. *International Journal of Heat and Mass Transfer*, **2011**, 54, 5183-5183	4.9	19
93	Thermal conductivity of hybrid graphene/silicon heterostructures. *Journal of Applied Physics*, **2013**, 114, 153518	2.5	18
92	Lone-Pair Electrons Do Not Necessarily Lead to Low Lattice Thermal Conductivity: An Exception of Two-Dimensional Penta-CN. *Journal of Physical Chemistry Letters*, **2018**, 9, 2474-2483	6.4	17
91	Molecular/cluster statistical thermodynamics methods to simulate quasi-static deformations at finite temperature. *International Journal of Solids and Structures*, **2008**, 45, 3918-3933	3.1	17
90	Unusual Thermal Boundary Resistance in Halide Perovskites: A Way To Tune Ultralow Thermal Conductivity for Thermoelectrics. *ACS Applied Materials & Interfaces*, **2019**, 11, 47507-47515	9.5	17
89	Anomalous pressure effect on the thermal conductivity of ZnO, GaN, and AlN from first-principles calculations. *Physical Review B*, **2018**, 98,	3.3	17
88	Extremely Low Thermal Conductivity of Polycrystalline Silicene. *Journal of Physical Chemistry C*, **2018**, 122, 9220-9228	3.8	16
87	Methodology for determining the electronic thermal conductivity of metals via direct nonequilibrium ab initio molecular dynamics. *Physical Review B*, **2016**, 94,	3.3	16
86	Strong Surface Orientation Dependent Thermal Transport in Si Nanowires. *Scientific Reports*, **2016**, 6, 24903	4.9	16
85	Mechanical behaviors of nanocrystalline Cu/SiC composites: An atomistic investigation. *Computational Materials Science*, **2017**, 129, 129-136	3.2	15
84	Unusual strain response of thermal transport in dimerized three-dimensional graphene. *Nanoscale*, **2018**, 10, 5229-5238	7.7	15
83	Thermal boundary conductance enhancement using experimentally achievable nanostructured interfaces - analytical study combined with molecular dynamics simulation. *Physical Chemistry Chemical Physics*, **2016**, 18, 16794-801	3.6	15

82	Predicting Elastic Properties of Materials from Electronic Charge Density Using 3D Deep Convolutional Neural Networks. *Journal of Physical Chemistry C*, **2020**, 124, 17262-17273	3.8	14
81	Surface Chemical Tuning of Phonon and Electron Transport in Free-Standing Silicon Nanowire Arrays. *Nano Letters*, **2016**, 16, 6364-6370	11.5	14
80	Ultrahigh thermal conductivity of carbon allotropes with correlations with the scaled Pugh ratio. *Journal of Materials Chemistry A*, **2019**, 7, 6259-6266	13	14
79	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	7.1	13
78	First-principles study on lattice thermal conductivity of thermoelectrics HgTe in different phases. *Journal of Applied Physics*, **2015**, 117, 245101	2.5	13
77	Giant effect of spin□lattice coupling on the thermal transport in two-dimensional ferromagnetic CrI3. *Journal of Materials Chemistry C*, **2020**, 8, 3520-3526	7.1	13
76	Strain-modulated electronic and thermal transport properties of two-dimensional O-silica. *Nanotechnology*, **2016**, 27, 265706	3.4	13
75	Unexpected anisotropy of (14,14,14)-Graphyne: A comprehensive study on the thermal transport properties of graphyne based nanomaterials. *Carbon*, **2019**, 143, 189-199	10.4	13
74	Lattice Thermal Conductivity Prediction Using Symbolic Regression and Machine Learning. *Journal of Physical Chemistry A*, **2021**, 125, 435-450	2.8	13
73	Development of a validated UPLC-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	12
72	Bond saturation significantly enhances thermal energy transport in two-dimensional pentagonal materials. *Nano Energy*, **2018**, 45, 1-9	17.1	12
71	Phonon transport in the ground state of two-dimensional silicon and germanium. *RSC Advances*, **2016**, 6, 69956-69965	3.7	12
70	Enhanced thermoelectric properties of the AGNR□GYNR heterojunctions. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2017**, 381, 3766-3772	2.3	11
69	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	11
68	An LC-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	3.5	11
67	Two-dimensional magnetic metal-organic frameworks with the Shastry-Sutherland lattice. *Chemical Science*, **2019**, 10, 10381-10387	9.4	11
66	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, 242101	3.4	10
65	The role of phonon-phonon and electron-phonon scattering in thermal transport in PdCoO. *Physical Chemistry Chemical Physics*, **2017**, 19, 21714-21721	3.6	9

64	Thermodynamic and Transport Properties of LiF and FLiBe Molten Salts with Deep Learning Potentials. *ACS Applied Materials & Interfaces*, **2021**, 13, 55367-55379	9.5	9
63	Spatial density neural network force fields with first-principles level accuracy and application to thermal transport. *Physical Review B*, **2020**, 102,	3.3	9
62	Enormous suppression of phonon transport in silicon nanowires with five-fold twin boundary. *Journal of Materials Chemistry A*, **2018**, 6, 18533-18542	13	9
61	Sustainable design rating system comparison using a life-cycle methodology. *Building and Environment*, **2017**, 126, 410-421	6.5	8
60	Machine Learning based prediction of noncentrosymmetric crystal materials. *Computational Materials Science*, **2020**, 183, 109792	3.2	8
59	Methodology Perspective of Computing Thermal Transport in Low-Dimensional Materials and Nanostructures: The Old and the New. *ACS Omega*, **2018**, 3, 3278-3284	3.9	8
58	Interfacial mixing during annealing of zinc oxide nanoparticle junctions. *Applied Physics Letters*, **2011**, 98, 211904	3.4	8
57	Unconventional thermal transport enhancement with large atom mass: a comparative study of 2D transition dichalcogenides. *2D Materials*, **2018**, 5, 015022	5.9	8
56	Electron-phonon interaction and superconductivity in the high-pressure cI16 phase of lithium from first principles. *Physical Chemistry Chemical Physics*, **2018**, 20, 27125-27130	3.6	8
55	Thermal conductivity of oxidized gamma-graphyne. *RSC Advances*, **2015**, 5, 65221-65226	3.7	7
54	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	4.9	7
53	Boundary scattering effect on the thermal conductivity of nanowires. *Semiconductor Science and Technology*, **2016**, 31, 074004	1.8	7
52	Improvement of Thermoelectricity Through Magnetic Interactions in Layered Cr2Ge2Te6. *Physica Status Solidi - Rapid Research Letters*, **2018**, 12, 1800172	2.5	7
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47	Dependence of phonon transport properties with stacking thickness in layered ZnO. *Journal Physics D: Applied Physics*, **2018**, 51, 315303	3	6

46	Ground state of bilayer h□silica: mechanical and electronic properties. *Nanotechnology*, **2015**, 26, 505702	3.4	6
45	Multi-scale analysis of AFM tip and surface interactions. *Chemical Engineering Science*, **2007**, 62, 3589-3594	4.4	6
44	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	3.4	6
43	Bidirectional effect of magnetic field on electronic thermal transport of metals from all-electron first-principles calculations. *Physical Review B*, **2016**, 94,	3.3	6
42	Accurate quantification of PGE in the polyposis in rat colon (Pirc) model by surrogate analyte-based UPLC-MS/MS. *Journal of Pharmaceutical and Biomedical Analysis*, **2018**, 148, 42-50	3.5	6
41	Molecular dynamics simulations of the effect of dislocations on the thermal conductivity of iron. *Journal of Applied Physics*, **2020**, 127, 045106	2.5	5
40	Air flow through carbon nanotube arrays. *Applied Physics Letters*, **2007**, 91, 131905	3.4	5
39	First Principles Investigation of Anomalous Pressure-Dependent Thermal Conductivity of Chalcopyrites. *Materials*, **2019**, 12,	3.5	5
38	The exceptionally high thermal conductivity after 'alloying' two-dimensional gallium nitride (GaN) and aluminum nitride (AlN). *Nanotechnology*, **2021**, 32, 135401	3.4	5
37	Probing the phonon mean free paths in dislocation core by molecular dynamics simulation. *Journal of Applied Physics*, **2021**, 129, 055103	2.5	5
36	Hyperelastic material modeling of graphene based on density functional calculations. *Proceedings in Applied Mathematics and Mechanics*, **2018**, 18, e201800419	0.2	5
35	Two-Channel Thermal Transport in Ordered-Disordered Superionic AgTe and Its Traditionally Contradictory Enhancement by Nanotwin Boundary. *Journal of Physical Chemistry Letters*, **2018**, 9, 5704-5709	6.4	5
34	Strong electron-phonon interaction retarding phonon transport in superconducting hydrogen sulfide at high pressures. *Physical Chemistry Chemical Physics*, **2018**, 20, 24222-24226	3.6	5
33	Decoupling thermal and electrical transport in □MgAgSb with synergic pressure and doping strategy. *Journal of Applied Physics*, **2019**, 125, 205105	2.5	4
32	Spin-dependent Seebeck effects in a graphene superlattice p-n junction with different shapes. *Journal of Physics Condensed Matter*, **2017**, 29, 405303	1.8	4
31	BaWOF: a mixed anion X-ray scintillator with excellent photoluminescence quantum efficiency. *Dalton Transactions*, **2020**, 49, 10734-10739	4.3	4
30	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	3.2	4
29	Perspective on multi-scale simulation of thermal transport in solids and interfaces. *Physical Chemistry Chemical Physics*, **2021**, 23, 1785-1801	3.6	4

28	Metavalent bonding induced abnormal phonon transport in diamondlike structures: Beyond conventional theory. *Physical Review B*, **2021**, 103,	3.3	4
27	Thermoelectric properties of four typical silicon allotropes. *Modelling and Simulation in Materials Science and Engineering*, **2018**, 26, 085006	2	4
26	High-Throughput Discovery of Novel Cubic Crystal Materials Using Deep Generative Neural Networks. *Advanced Science*, **2021**, 8, e2100566	13.6	4
25	Cluster Statistical Thermodynamics (CST) To Efficiently Calculate Quasi-Static Deformation at Finite Temperature Based on Molecular Potential **2007**, 163-170		4
24	Doping Induced Abnormal Contraction and Significant Reduction of Lattice Thermal Conductivity of Open Framework Si24. *ES Energy & Environments*, **2018**,	2.9	3
23	High-Throughput Computation of New Carbon Allotropes with Diverse Hybridization and Ultrahigh Hardness. *Crystals*, **2021**, 11, 783	2.3	3
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21	Phonon scattering in the complex strain field of a dislocation in PbTe. *Journal of Materials Chemistry C*, **2021**, 9, 8506-8514	7.1	3
20	Analytical study on the size effect of phonon spectral energy density resolution. *Computational Materials Science*, **2017**, 132, 6-9	3.2	2
19	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	2.4	2
18	Insight of the thermal conductivity of ?-iron at Earth's core conditions from the newly developed direct ab initio methodology. *Journal of Applied Physics*, **2019**, 125, 045102	2.5	2
17	Thermal transport properties of monolayer phosphorene: a mini-review of theoretical studies. *Frontiers in Energy*, **2018**, 12, 87-96	2.6	2
16	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	4.1	2
15	Diverse Thermal Transport Properties of Two-Dimensional Materials: A Comparative Review **2016**,		2
14	Fluoride-Based Anion Doping: A New Strategy for Improving the Performance of Protonic Ceramic Conductors of the Form BaZrO3. *ChemElectroChem*, **2020**, 7, 2242-2247	4.3	2
13	Exploration of exciton behavior in atomically thin WS2 layers by ionic gating. *Applied Physics Letters*, **2018**, 113, 013104	3.4	2
12	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	1.8	1
11	Tailoring thermal conductivity of AlN films by periodically aligned surface nano-grooves. *Applied Physics Letters*, **2016**, 109, 133107	3.4	1

10	Enhanced Two-Photon Absorption in Two Triphenylamine-Based All-Organic Compounds. *Journal of Physical Chemistry A*, **2021**, 125, 1870-1879	2.8	1
9	The lattice thermal conductivity in monolayers group-VA: from elements to binary compounds. *Materials Research Express*, **2021**, 8, 075007	1.7	1
8	Energetic Barriers of Gas Permeation across Nanoporous Graphene. *ACS Applied Materials & Interfaces*, **2021**, 13, 39701-39710	9.5	1
7	Hydrothermal syntheses and crystal structures of molybdenum tellurites. *Journal of Solid State Chemistry*, **2020**, 287, 121317	3.3	0
6	High-throughput computation of novel ternary B□□N structures and carbon allotropes with electronic-level insights into superhard materials from machine learning. *Journal of Materials Chemistry A*, **2021**, 9, 27596-27614	13	0
5	Large scale dataset of real space electronic charge density of cubic inorganic materials from density functional theory (DFT) calculations.. *Scientific Data*, **2022**, 9, 59	8.2	0
4	Molecular Dynamics Simulation of Thermal Conductivity of Diamondoid Crystals. *Materials Research Society Symposia Proceedings*, **2007**, 1022, 1		
3	Two-dimensional silicon. *Series in Materials Science and Engineering*, **2017**, 43-76		
2	Si nanowires for evolutionary nanotechnology. *Series in Materials Science and Engineering*, **2017**, 515-536		
1	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	