Xiaokun Gu

List of Publications by Year
in descending order

48 papers	3,597 citations	218677 26 h-index	223800 46 g-index
48 all docs	48 docs citations	48 times ranked	4856 citing authors

#	Article	IF	Citations
1	Impact of thermostat on interfacial thermal conductance prediction from non-equilibrium molecular dynamics simulations. Chinese Physics B, 2022, 31, 056301.	1.4	10
2	High-temperature phonon transport properties of SnSe from machine-learning interatomic potential. Journal of Physics Condensed Matter, 2021, 33, 405401.	1.8	24
3	GPU_PBTE: an efficient solver for three and four phonon scattering rates on graphics processing units. Journal of Physics Condensed Matter, 2021, 33, 495901.	1.8	6
4	The energy efficiency of interfacial solar desalination. Applied Energy, 2021, 302, 117581.	10.1	60
5	Thermal conductivity prediction by atomistic simulation methods: Recent advances and detailed comparison. Journal of Applied Physics, 2021, 130, .	2.5	36
6	A minimal Tersoff potential for diamond silicon with improved descriptions of elastic and phonon transport properties. Journal of Physics Condensed Matter, 2020, 32, 135901.	1.8	9
7	Anomalous thermal transport in metallic transition-metal nitrides originated from strong electronâ€“phonon interactions. Materials Today Physics, 2020, 15, 100256.	6.0	22
8	Thermal conductivity of silicon at elevated temperature: Role of four-phonon scattering and electronic heat conduction. International Journal of Heat and Mass Transfer, 2020, 160, 120165.	4.8	21
9	Monitoring anharmonic phonon transport across interfaces in one-dimensional lattice chains. Physical Review E, 2020, 101, 022133.	2.1	8
10	Unification of nonequilibrium molecular dynamics and the mode-resolved phonon Boltzmann equation for thermal transport simulations. Physical Review B, 2020, 101, .	3.2	49
11	Seeking for Low Thermal Conductivity Atomic Configurations in SiGe Alloys with Bayesian Optimization. ES Energy & Environments, 2020, , .	1.1	14
12	Revisiting phonon-phonon scattering in single-layer graphene. Physical Review B, 2019, 100, .	3.2	71
13	Thermal conductivity of MoS2/MoSe2 heterostructures: The role of lattice mismatch, interlayer rotation and species intermixing. International Journal of Heat and Mass Transfer, 2019, 143, 118583.	4.8	17
14	A scattering rate model for accelerated evaluation of lattice thermal conductivity bypassing anharmonic force constants. Journal of Applied Physics, 2019, 125, .	2.5	6
15	Thermal conductivity of single-layer MoS2(1âˆ’x)Se2x alloys from molecular dynamics simulations with a machine-learning-based interatomic potential. Computational Materials Science, 2019, 165, 74-81.	3.0	46
16	<i>Colloquium</i>: Phononic thermal properties of two-dimensional materials. Reviews of Modern Physics, 2018, 90, .	45.6	238
17	Electronic band structure of carbon honeycombs. Materials Today Physics, 2018, 5, 72-77.	6.0	5
18	Thermal conductivity of hexagonal Si, Ge, and Si1-xGex alloys from first-principles. Journal of Applied Physics, 2018, 123, .	2.5	12

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19	Anisotropic thermal transport in van der Waals layered alloys WSe2(1-<i>x</i>)Te2<i>x</i>. Applied Physics Letters, 2018, 112, .	3.3	32
20	A Review of Simulation Methods in Micro/Nanoscale Heat Conduction. ES Energy & Environments, 2018, , .	1.1	78
21	HIGH TEMPERATURE THERMAL CONDUCTIVITY OF SILICON FROM MACHINE-LEARNING-BASED INTERATOMIC POTENTIAL. , 2018, , .		0
22	On the influence of junction structures on the mechanical and thermal properties of carbon honeycombs. Carbon, 2017, 119, 278-286.	10.3	56
23	Bottom-up Design of Three-Dimensional Carbon-Honeycomb with Superb Specific Strength and High Thermal Conductivity. Nano Letters, 2017, 17, 179-185.	9.1	95
24	Thermal conductivity modeling of hybrid organic-inorganic crystals and superlattices. Nano Energy, 2017, 41, 394-407.	16.0	32
25	Probing Anisotropic Thermal Conductivity of Transition Metal Dichalcogenides MX₂ (M =) Tj ETQq1 1 0.784314 rgBT /Over	21.0	163
26	Effect of the accuracy of interatomic force constants on the prediction of lattice thermal conductivity. Computational Materials Science, 2017, 138, 368-376.	3.0	15
27	Temperature Dependence of Anisotropic Thermalâ€Conductivity Tensor of Bulk Black Phosphorus. Advanced Materials, 2017, 29, 1603297.	21.0	89
28	Revealing the Origins of 3D Anisotropic Thermal Conductivities of Black Phosphorus. Advanced Electronic Materials, 2016, 2, 1600040.	5.1	85
29	Lattice thermal conductivity of organic-inorganic hybrid perovskite CH3NH3PbI3. Applied Physics Letters, 2016, 108, .	3.3	97
30	Layer thickness-dependent phonon properties and thermal conductivity of MoS2. Journal of Applied Physics, 2016, 119, .	2.5	136
31	Measurement Techniques for Thermal Conductivity and Interfacial Thermal Conductance of Bulk and Thin Film Materials. Journal of Electronic Packaging, Transactions of the ASME, 2016, 138, .	1.8	328
32	Phonon transport in single-layerMo1â^'xWxS2alloy embedded withWS2nanodomains. Physical Review B, 2016, 94, .	3.2	18
33	Anisotropic Tuning of Graphite Thermal Conductivity by Lithium Intercalation. Journal of Physical Chemistry Letters, 2016, 7, 4744-4750.	4.6	69
34	Black Phosphorus: Revealing the Origins of 3D Anisotropic Thermal Conductivities of Black Phosphorus (Adv. Electron. Mater. 5/2016). Advanced Electronic Materials, 2016, 2, .	5.1	4
35	PHONON TRANSPORT AND THERMAL CONDUCTIVITY IN TWO-DIMENSIONAL MATERIALS. Annual Review of Heat Transfer, 2016, 19, 1-65.	1.0	57
36	Phonon transmission across<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Mg</mml:mi><mml:mn>2</mml:mn></mml A first-principles-based atomistic Green's function study. Physical Review B, 2015, 91, .	3.2	16

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37	Anisotropic Thermal Transport in Organicâ€"Inorganic Hybrid Crystal Î²-ZnTe(en)0.5. Journal of Physical Chemistry C, 2015, 119, 28300-28308.	3.1	16
38	First-principles prediction of phononic thermal conductivity of silicene: A comparison with graphene. Journal of Applied Physics, 2015, 117, .	2.5	204
39	Mechanical and thermal properties of nanomaterials at sub-50nm dimensions characterized using coherent EUV beams. , 2015, , .		0
40	A new regime of nanoscale thermal transport: Collective diffusion increases dissipation efficiency. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 4846-4851.	7.1	170
41	Flexible n-type thermoelectric materials by organic intercalation of layered transition metalÂdichalcogenide TiS2. Nature Materials, 2015, 14, 622-627.	27.5	612
42	Dielectric Mismatch Mediates Carrier Mobility in Organic-Intercalated Layered TiS₂. Nano Letters, 2015, 15, 6302-6308.	9.1	62
43	A New Regime of Nanoscale Thermal Transport: Collective Diffusion Counteracts Dissipation Inefficiency. Springer Proceedings in Physics, 2015, , 341-344.	0.2	3
44	Phonon transport in single-layer transition metal dichalcogenides: A first-principles study. Applied Physics Letters, 2014, 105, .	3.3	309
45	Stable planar single-layer hexagonal silicene under tensile strain and its anomalous Poisson's ratio. Applied Physics Letters, 2014, 104, 081902.	3.3	49
46	Simultaneous measurement of thermal conductivity and heat capacity of bulk and thin film materials using frequency-dependent transient thermoreflectance method. Review of Scientific Instruments, 2013, 84, 034902.	1.3	120
47	Shape dependence of slip length on patterned hydrophobic surfaces. Applied Physics Letters, 2011, 99, .	3.3	13
48	Thermal conductivity of dielectric nanowires with different cross-section shapes. Chinese Physics B, 2007, 16, 3777-3782.	1.3	15