Zheyong Fan

List of Publications by Year
in descending order

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65 papers	2,394 citations	201385 27 h-index	214527 47 g-index
67 all docs	67 docs citations	67 times ranked	2000 citing authors

#	Article	IF	Citations
1	Force and heat current formulas for many-body potentials in molecular dynamics simulations with applications to thermal conductivity calculations. Physical Review B, 2015, 92, .	1.1	215
2	Efficient molecular dynamics simulations with many-body potentials on graphics processing units. Computer Physics Communications, 2017, 218, 10-16.	3.0	126
3	Influence of thermostatting on nonequilibrium molecular dynamics simulations of heat conduction in solids. Journal of Chemical Physics, 2019, 151, 234105.	1.2	126
4	Graphene-nanotube 3D networks: intriguing thermal and mechanical properties. Journal of Materials Chemistry, 2012, 22, 1435-1444.	6.7	118
5	Thermal conductivity decomposition in two-dimensional materials: Application to graphene. Physical Review B, 2017, 95, .	1.1	113
6	Neuroevolution machine learning potentials: Combining high accuracy and low cost in atomistic simulations and application to heat transport. Physical Review B, 2021, 104, .	1.1	101
7	Amorphized graphene: A stiff material with low thermal conductivity. Carbon, 2016, 103, 318-326.	5.4	82
8	N-graphdiyne two-dimensional nanomaterials: Semiconductors with low thermal conductivity and high stretchability. Carbon, 2018, 137, 57-67.	5.4	82
9	Homogeneous nonequilibrium molecular dynamics method for heat transport and spectral decomposition with many-body potentials. Physical Review B, 2019, 99, .	1.1	77
10	Mechanical properties of grafold: a demonstration of strengthened graphene. Nanotechnology, 2011, 22, 405701.	1.3	75
11	Multiscale modeling of polycrystalline graphene: A comparison of structure and defect energies of realistic samples from phase field crystal models. Physical Review B, 2016, 94, .	1.1	72
12	Revisiting phonon-phonon scattering in single-layer graphene. Physical Review B, 2019, 100, .	1.1	71
13	Equivalence of the equilibrium and the nonequilibrium molecular dynamics methods for thermal conductivity calculations: From bulk to nanowire silicon. Physical Review B, 2018, 97, .	1.1	55
14	Thermal transport in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> from molecular dynamics using different empirical potentials. Physical Review B, 2019, 99, .	1.1	55
15	Anderson localization in two-dimensional graphene with short-range disorder: One-parameter scaling and finite-size effects. Physical Review B, 2014, 89, .	1.1	49
16	Unification of nonequilibrium molecular dynamics and the mode-resolved phonon Boltzmann equation for thermal transport simulations. Physical Review B, 2020, 101, .	1.1	49
17	Accelerated molecular dynamics force evaluation on graphics processing units for thermal conductivity calculations. Computer Physics Communications, 2013, 184, 1414-1425.	3.0	47
18	Kapitza thermal resistance across individual grain boundaries in graphene. Carbon, 2017, 125, 384-390.	5.4	46

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19	Linear scaling quantum transport methodologies. Physics Reports, 2021, 903, 1-69.	10.3	46
20	Searching for the best thermoelectrics through the optimization of transport distribution function. Journal of Applied Physics, 2011, 109, .	1.1	36
21	Thermal conductivity prediction by atomistic simulation methods: Recent advances and detailed comparison. Journal of Applied Physics, 2021, 130, .	1.1	36
22	Mechanical Properties of Graphene Nanobuds: A Molecular Dynamics Study. Current Nanoscience, 2012, 8, 89-96.	0.7	31
23	Heat transport in pristine and polycrystalline single-layer hexagonal boron nitride. Physical Chemistry Chemical Physics, 2018, 20, 24602-24612.	1.3	31
24	Spectral decomposition of thermal conductivity: Comparing velocity decomposition methods in homogeneous molecular dynamics simulations. Physical Review B, 2021, 103, .	1.1	30
25	Nonperturbative phonon scatterings and the two-channel thermal transport in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Tl</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> Physical Review B, 2021, 103, .	1.1	30
26	Enhanced thermoelectric performance in three-dimensional superlattice of topological insulator thin films. Nanoscale Research Letters, 2012, 7, 570.	3.1	29
27	Structure and Pore Size Distribution in Nanoporous Carbon. Chemistry of Materials, 2022, 34, 617-628.	3.2	29
28	Efficient linear-scaling quantum transport calculations on graphics processing units and applications on electron transport in graphene. Computer Physics Communications, 2014, 185, 28-39.	3.0	28
29	Thermal and electronic transport characteristics of highly stretchable graphene kirigami. Nanoscale, 2017, 9, 16329-16341.	2.8	28
30	Bimodal Grain-Size Scaling of Thermal Transport in Polycrystalline Graphene from Large-Scale Molecular Dynamics Simulations. Nano Letters, 2017, 17, 5919-5924.	4.5	28
31	Thermal transport properties of single-layer black phosphorus from extensive molecular dynamics simulations. Modelling and Simulation in Materials Science and Engineering, 2018, 26, 085001.	0.8	28
32	Improving the accuracy of the neuroevolution machine learning potential for multi-component systems. Journal of Physics Condensed Matter, 2022, 34, 125902.	0.7	28
33	Anomalous thermal conductivity enhancement in low dimensional resonant nanostructures due to imperfections. Nanoscale, 2021, 13, 10010-10015.	2.8	26
34	Time reversal symmetry breaking holographic superconductor in constant external magnetic field. Physical Review D, 2009, 80, .	1.6	24
35	A molecular dynamics investigation of the mechanical properties of graphene nanochains. Journal of Materials Chemistry, 2012, 22, 9798.	6.7	23
36	Silicon and silicon-nitrogen impurities in graphene: Structure, energetics, and effects on electronic transport. Physical Review B, 2015, 92, .	1.1	23

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37	Knitted graphene-nanoribbon sheet: a mechanically robust structure. Nanoscale, 2012, 4, 785-791.	2.8	22
38	Energetics and structure of grain boundary triple junctions in graphene. Scientific Reports, 2017, 7, 4754.	1.6	22
39	Thermal conductivity reduction in carbon nanotube by fullerene encapsulation: A molecular dynamics study. Carbon, 2020, 161, 800-808.	5.4	22
40	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>d</mml:mi></mml:math>-wave holographic superconductor vortex lattice and non-Abelian holographic superconductor droplet. Physical Review D, 2010, 82, .	1.6	18
41	Inter-layer and intra-layer heat transfer in bilayer/monolayer graphene van der Waals heterostructure: Is there a Kapitza resistance analogous?. Applied Physics Letters, 2018, 112, .	1.5	18
42	Ultrahigh Convergent Thermal Conductivity of Carbon Nanotubes from Comprehensive Atomistic Modeling. Physical Review Letters, 2021, 127, 025902.	2.9	18
43	Enhanced thermoelectric performance in graphitic ZnO (0001) nanofilms. Journal of Applied Physics, 2013, 113, .	1.1	14
44	Obtaining localization properties efficiently using the Kubo-Greenwood formalism. Physical Review B, 2014, 89, .	1.1	14
45	Efficient Calculation of the Lattice Thermal Conductivity by Atomistic Simulations with Ab Initio Accuracy. Advanced Theory and Simulations, 2022, 5, .	1.3	14
46	Defect-activated self-assembly of multilayered graphene paper: a mechanically robust architecture with high strength. Journal of Materials Chemistry A, 2013, 1, 2002-2010.	5.2	12
47	Nonlinear conductivity of a holographic superconductor under constant electric field. Physical Review D, 2017, 95, .	1.6	11
48	Methodology Perspective of Computing Thermal Transport in Low-Dimensional Materials and Nanostructures: The Old and the New. ACS Omega, 2018, 3, 3278-3284.	1.6	11
49	Mechanical properties of grafold: a demonstration of strengthened graphene. Nanotechnology, 2011, 22, 479501.	1.3	10
50	Phase-field crystal model for heterostructures. Physical Review B, 2019, 100, .	1.1	10
51	Characteristic length of a holographic superconductor with<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>d</mml:mi></mml:math>-wave gap. Physical Review D, 2010, 82, .	1.6	9
52	Electronic and transport properties in geometrically disordered graphene antidot lattices. Physical Review B, 2015, 91, .	1.1	9
53	A minimal Tersoff potential for diamond silicon with improved descriptions of elastic and phonon transport properties. Journal of Physics Condensed Matter, 2020, 32, 135901.	0.7	9
54	Interpretation of apparent thermal conductivity in finite systems from equilibrium molecular dynamics simulations. Physical Review B, 2021, 103, .	1.1	9

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55	Size effect and transient phonon transport mechanism in approach-to-equilibrium molecular dynamics simulations. Physical Review B, 2022, 105, .	1.1	8
56	Heat transport across graphene/hexagonal-BN tilted grain boundaries from phase-field crystal model and molecular dynamics simulations. Journal of Applied Physics, 2021, 130, .	1.1	8
57	GPUQT: An efficient linear-scaling quantum transport code fully implemented on graphics processing units. Computer Physics Communications, 2018, 230, 113-120.	3.0	7
58	Braid matrices and quantum gates for Ising anyons topological quantum computation. European Physical Journal B, 2010, 74, 419-427.	0.6	6
59	Dominant source of disorder in graphene: charged impurities or ripples?. 2D Materials, 2017, 4, 025004.	2.0	6
60	GPU_PBTE: an efficient solver for three and four phonon scattering rates on graphics processing units. Journal of Physics Condensed Matter, 2021, 33, 495901.	0.7	6
61	Scattering from spin-polarized charged impurities in graphene. Physical Review B, 2017, 95, .	1.1	5
62	No-ghost theorem for the bosonic Nappi-Witten string. Physical Review D, 2009, 80, .	1.6	3
63	Grain extraction and microstructural analysis method for two-dimensional poly and quasicrystalline solids. Physical Review Materials, 2018, 2, .	0.9	3
64	Exactly equivalent thermal conductivity in finite systems from equilibrium and nonequilibrium molecular dynamics simulations. Physica E: Low-Dimensional Systems and Nanostructures, 2022, 144, 115410.	1.3	2
65	Structural and Electronic Properties of c-BC2N Supper Hard Material: an Ab-Initio Study. Materials Science Forum, 2011, 694, 676-681.	0.3	0