Zheyong Fan

List of Publications by Citations

62 papers	1,454 citations	22 h-index	36 g-index
67 ext. papers	1,892 ext. citations	4.8 avg, IF	5.04 L-index

#	Paper	IF	Citations
62	Force and heat current formulas for many-body potentials in molecular dynamics simulations with applications to thermal conductivity calculations. *Physical Review B*, **2015**, 92,	3.3	144
61	Graphene-nanotube 3D networks: intriguing thermal and mechanical properties. *Journal of Materials Chemistry*, **2012**, 22, 1435-1444		101
60	Thermal conductivity decomposition in two-dimensional materials: Application to graphene. *Physical Review B*, **2017**, 95,	3.3	78
59	Mechanical properties of grafold: a demonstration of strengthened graphene. *Nanotechnology*, **2011**, 22, 405701	3.4	72
58	Efficient molecular dynamics simulations with many-body potentials on graphics processing units. *Computer Physics Communications*, **2017**, 218, 10-16	4.2	70
57	Amorphized graphene: A stiff material with low thermal conductivity. *Carbon*, **2016**, 103, 318-326	10.4	70
56	N-graphdiyne two-dimensional nanomaterials: Semiconductors with low thermal conductivity and high stretchability. *Carbon*, **2018**, 137, 57-67	10.4	67
55	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,	3.3	56
54	Influence of thermostatting on nonequilibrium molecular dynamics simulations of heat conduction in solids. *Journal of Chemical Physics*, **2019**, 151, 234105	3.9	56
53	Equivalence of the equilibrium and the nonequilibrium molecular dynamics methods for thermal conductivity calculations: From bulk to nanowire silicon. *Physical Review B*, **2018**, 97,	3.3	38
52	Anderson localization in two-dimensional graphene with short-range disorder: One-parameter scaling and finite-size effects. *Physical Review B*, **2014**, 89,	3.3	34
51	Revisiting phonon-phonon scattering in single-layer graphene. *Physical Review B*, **2019**, 100,	3.3	33
50	Kapitza thermal resistance across individual grain boundaries in graphene. *Carbon*, **2017**, 125, 384-390	10.4	33
49	Thermal transport in MoS2 from molecular dynamics using different empirical potentials. *Physical Review B*, **2019**, 99,	3.3	31
48	Accelerated molecular dynamics force evaluation on graphics processing units for thermal conductivity calculations. *Computer Physics Communications*, **2013**, 184, 1414-1425	4.2	30
47	Homogeneous nonequilibrium molecular dynamics method for heat transport and spectral decomposition with many-body potentials. *Physical Review B*, **2019**, 99,	3.3	29
46	Searching for the best thermoelectrics through the optimization of transport distribution function. *Journal of Applied Physics*, **2011**, 109, 073713	2.5	29

45	Efficient linear-scaling quantum transport calculations on graphics processing units and applications on electron transport in graphene. *Computer Physics Communications*, **2014**, 185, 28-39	4.2	26
44	Mechanical Properties of Graphene Nanobuds: A Molecular Dynamics Study. *Current Nanoscience*, **2012**, 8, 89-96	1.4	26
43	Enhanced thermoelectric performance in three-dimensional superlattice of topological insulator thin films. *Nanoscale Research Letters*, **2012**, 7, 570	5	24
42	Time reversal symmetry breaking holographic superconductor in constant external magnetic field. *Physical Review D*, **2009**, 80,	4.9	23
41	A molecular dynamics investigation of the mechanical properties of graphene nanochains. *Journal of Materials Chemistry*, **2012**, 22, 9798		22
40	Bimodal Grain-Size Scaling of Thermal Transport in Polycrystalline Graphene from Large-Scale Molecular Dynamics Simulations. *Nano Letters*, **2017**, 17, 5919-5924	11.5	21
39	Silicon and silicon-nitrogen impurities in graphene: Structure, energetics, and effects on electronic transport. *Physical Review B*, **2015**, 92,	3.3	21
38	Unification of nonequilibrium molecular dynamics and the mode-resolved phonon Boltzmann equation for thermal transport simulations. *Physical Review B*, **2020**, 101,	3.3	21
37	Thermal and electronic transport characteristics of highly stretchable graphene kirigami. *Nanoscale*, **2017**, 9, 16329-16341	7.7	19
36	Linear scaling quantum transport methodologies. *Physics Reports*, **2021**, 903, 1-69	27.7	19
35	Thermal transport properties of single-layer black phosphorus from extensive molecular dynamics simulations. *Modelling and Simulation in Materials Science and Engineering*, **2018**, 26, 085001	2	18
34	Heat transport in pristine and polycrystalline single-layer hexagonal boron nitride. *Physical Chemistry Chemical Physics*, **2018**, 20, 24602-24612	3.6	18
33	Knitted graphene-nanoribbon sheet: a mechanically robust structure. *Nanoscale*, **2012**, 4, 785-91	7.7	16
32	d-wave holographic superconductor vortex lattice and non-Abelian holographic superconductor droplet. *Physical Review D*, **2010**, 82,	4.9	15
31	Energetics and structure of grain boundary triple junctions in graphene. *Scientific Reports*, **2017**, 7, 4754	4.9	14
30	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, 233104	3.4	13
29	Obtaining localization properties efficiently using the Kubo-Greenwood formalism. *Physical Review B*, **2014**, 89,	3.3	13
28	Defect-activated self-assembly of multilayered graphene paper: a mechanically robust architecture with high strength. *Journal of Materials Chemistry A*, **2013**, 1, 2002-2010	13	12

27	Thermal conductivity reduction in carbon nanotube by fullerene encapsulation: A molecular dynamics study. *Carbon*, **2020**, 161, 800-808	10.4	9
26	Nonlinear conductivity of a holographic superconductor under constant electric field. *Physical Review D*, **2017**, 95,	4.9	9
25	Mechanical properties of grafold: a demonstration of strengthened graphene. *Nanotechnology*, **2011**, 22, 479501	3.4	9
24	Spectral decomposition of thermal conductivity: Comparing velocity decomposition methods in homogeneous molecular dynamics simulations. *Physical Review B*, **2021**, 103,	3.3	9
23	Nonperturbative phonon scatterings and the two-channel thermal transport in Tl3VSe4. *Physical Review B*, **2021**, 103,	3.3	9
22	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
21	Electronic and transport properties in geometrically disordered graphene antidot lattices. *Physical Review B*, **2015**, 91,	3.3	8
20	Enhanced thermoelectric performance in graphitic ZnO (0001) nanofilms. *Journal of Applied Physics*, **2013**, 113, 083705	2.5	7
19	GPUQT: An efficient linear-scaling quantum transport code fully implemented on graphics processing units. *Computer Physics Communications*, **2018**, 230, 113-120	4.2	7
18	Dominant source of disorder in graphene: charged impurities or ripples?. *2D Materials*, **2017**, 4, 025004	5.9	6
17	Characteristic length of a holographic superconductor with d-wave gap. *Physical Review D*, **2010**, 82,	4.9	6
16	Ultrahigh Convergent Thermal Conductivity of Carbon Nanotubes from Comprehensive Atomistic Modeling. *Physical Review Letters*, **2021**, 127, 025902	7.4	6
15	Neuroevolution machine learning potentials: Combining high accuracy and low cost in atomistic simulations and application to heat transport. *Physical Review B*, **2021**, 104,	3.3	6
14	Scattering from spin-polarized charged impurities in graphene. *Physical Review B*, **2017**, 95,	3.3	5
13	Phase-field crystal model for heterostructures. *Physical Review B*, **2019**, 100,	3.3	5
12	Thermal conductivity prediction by atomistic simulation methods: Recent advances and detailed comparison. *Journal of Applied Physics*, **2021**, 130, 210902	2.5	5
11	Anomalous thermal conductivity enhancement in low dimensional resonant nanostructures due to imperfections. *Nanoscale*, **2021**, 13, 10010-10015	7.7	4
10	No-ghost theorem for the bosonic Nappi-Witten string. *Physical Review D*, **2009**, 80,	4.9	3

9	Structure and Pore Size Distribution in Nanoporous Carbon. *Chemistry of Materials*, **2022**, 34, 617-628	9.6	3
8	Grain extraction and microstructural analysis method for two-dimensional poly and quasicrystalline solids. *Physical Review Materials*, **2018**, 2,	3.2	3
7	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	3
6	GPU_PBTE: an efficient solver for three and four phonon scattering rates on graphics processing units. *Journal of Physics Condensed Matter*, **2021**, 33,	1.8	3
5	Interpretation of apparent thermal conductivity in finite systems from equilibrium molecular dynamics simulations. *Physical Review B*, **2021**, 103,	3.3	3
4	Braid matrices and quantum gates for Ising anyons topological quantum computation. *European Physical Journal B*, **2010**, 74, 419-427	1.2	2
3	Efficient Calculation of the Lattice Thermal Conductivity by Atomistic Simulations with Ab Initio Accuracy. *Advanced Theory and Simulations*,2100217	3.5	2
2	Heat transport across graphene/hexagonal-BN tilted grain boundaries from phase-field crystal model and molecular dynamics simulations. *Journal of Applied Physics*, **2021**, 130, 235102	2.5	1
1	Structural and Electronic Properties of c-BC2N Supper Hard Material: an Ab-Initio Study. *Materials Science Forum*, **2011**, 694, 676-681	0.4	