Guang-Zhao Qin

List of Publications by Year
in descending order

81 papers	3,357 citations	185998 28 h-index	149479 56 g-index
83 all docs	83 docs citations	83 times ranked	3165 citing authors

#	Article	IF	Citations
1	Anisotropic intrinsic lattice thermal conductivity of phosphorene from first principles. Physical Chemistry Chemical Physics, 2015, 17, 4854-4858.	1.3	379
2	Diverse anisotropy of phonon transport in two-dimensional group IVâ€"VI compounds: A comparative study. Nanoscale, 2016, 8, 11306-11319.	2.8	234
3	Thermal conductivity of silicene calculated using an optimized Stillinger-Weber potential. Physical Review B, 2014, 89, .	1.1	213
4	Hinge-like structure induced unusual properties of black phosphorus and new strategies to improve the thermoelectric performance. Scientific Reports, 2014, 4, 6946.	1.6	202
5	Disparate Strain Dependent Thermal Conductivity of Two-dimensional Penta-Structures. Nano Letters, 2016, 16, 3831-3842.	4.5	183
6	Large tunability of lattice thermal conductivity of monolayer silicene via mechanical strain. Physical Review B, 2016, 93, .	1.1	166
7	Tinselenidene: a Two-dimensional Auxetic Material with Ultralow Lattice Thermal Conductivity and Ultrahigh Hole Mobility. Scientific Reports, 2016, 6, 19830.	1.6	155
8	Orbitally driven low thermal conductivity of monolayer gallium nitride (GaN) with planar honeycomb structure: a comparative study. Nanoscale, 2017, 9, 4295-4309.	2.8	155
9	Resonant bonding driven giant phonon anharmonicity and low thermal conductivity of phosphorene. Physical Review B, 2016, 94, .	1.1	114
10	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:math law. Physical Review B, 2017, 95, .	1.1	101
11	External electric field driving the ultra-low thermal conductivity of silicene. Nanoscale, 2017, 9, 7227-7234.	2.8	69
12	First-principles study of electronic, optical and thermal transport properties of group IIIâ€"VI monolayer MX (Mâ€‰=â€‰Ga, In; Xâ€‰=â€‰S, Se). Journal of Applied Physics, 2019, 125, .	1.1	61
13	Thermal transport properties of GaN with biaxial strain and electron-phonon coupling. Journal of Applied Physics, 2020, 127, .	1.1	59
14	Negative Poissonâ€™s ratio in two-dimensional honeycomb structures. Npj Computational Materials, 2020, 6, .	3.5	56
15	Low thermal conductivity of monolayer ZnO and its anomalous temperature dependence. Physical Chemistry Chemical Physics, 2017, 19, 12882-12889.	1.3	55
16	Lone-pair electrons induced anomalous enhancement of thermal transport in strained planar two-dimensional materials. Nano Energy, 2018, 50, 425-430.	8.2	55
17	Nontrivial contribution of FrÃ¶hlich electron-phonon interaction to lattice thermal conductivity of wurtzite GaN. Applied Physics Letters, 2016, 109, .	1.5	53
18	Insight into the collective vibrational modes driving ultralow thermal conductivity of perovskite solar cells. Physical Review B, 2016, 94, .	1.1	52

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19	Accelerating evaluation of converged lattice thermal conductivity. Npj Computational Materials, 2018, 4, .	3.5	50
20	Origin of anisotropic negative Poisson's ratio in graphene. Nanoscale, 2018, 10, 10365-10370.	2.8	43
21	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:m 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:m hybridization: An <i>ab initio</i> study. Physical Review B, 2017, 95, .	1.1	42
22	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.	2.1	38
23	Exploring T-carbon for energy applications. Nanoscale, 2019, 11, 5798-5806.	2.8	38
24	Two-dimensional Al2I2Se2: A promising anisotropic thermoelectric material. Journal of Alloys and Compounds, 2021, 876, 160191.	2.8	37
25	Thermal Transport in Phosphorene. Small, 2018, 14, e1702465.	5.2	36
26	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.	1.4	34
27	Thermal conductivity of polydisperse hexagonal BN/polyimide composites: Iterative EMT model and machine learning based on first principles investigation. Chemical Engineering Journal, 2022, 437, 135438.	6.6	32
28	Giant effect of spinâ€“lattice coupling on the thermal transport in two-dimensional ferromagnetic CrI₃. Journal of Materials Chemistry C, 2020, 8, 3520-3526.	2.7	31
29	Disparate strain response of the thermal transport properties of bilayer penta-graphene as compared to that of monolayer penta-graphene. Physical Chemistry Chemical Physics, 2019, 21, 15647-15655.	1.3	28
30	Metric for strong intrinsic fourth-order phonon anharmonicity. Physical Review B, 2017, 95, .	1.1	26
31	Two-dimensional layered MSi₂N₄ (M = Mo, W) as promising thermal management materials: a comparative study. Physical Chemistry Chemical Physics, 2022, 24, 3086-3093.	1.3	24
32	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.	2.6	23
33	Measurements and calculations of thermal conductivity for liquid n-octane and n-decane. Fluid Phase Equilibria, 2021, 533, 112940.	1.4	23
34	The exceptionally high thermal conductivity after â€˜alloyingâ€™ two-dimensional gallium nitride (GaN) and aluminum nitride (AlN). Nanotechnology, 2021, 32, 135401.	1.3	22
35	Measurement and modeling of thermal conductivity for short chain methyl esters: Methyl butyrate and methyl caproate. Journal of Chemical Thermodynamics, 2021, 159, 106486.	1.0	22
36	Efficient thermal conductivity modulation by manipulating interlayer interactions: A comparative study of bilayer graphene and graphite. Journal of Applied Physics, 2019, 126, .	1.1	21

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37	Two-dimensional magnetic metalâ€"organic frameworks with the Shastry-Sutherland lattice. Chemical Science, 2019, 10, 10381-10387.	3.7	21
38	Behavior of aluminum adsorption and incorporation at GaN(0001) surface: First-principles study. Journal of Applied Physics, 2013, 114, .	1.1	20
39	Phonon transport in the ground state of two-dimensional silicon and germanium. RSC Advances, 2016, 6, 69956-69965.	1.7	20
40	Strain-modulated electronic and thermal transport properties of two-dimensional O-silica. Nanotechnology, 2016, 27, 265706.	1.3	18
41	Thermal conductivity measurements for long-chain n-alkanes at evaluated temperature and pressure: n-dodecane and n-tetradecane. Journal of Chemical Thermodynamics, 2021, 162, 106566.	1.0	18
42	Methodology for determining the electronic thermal conductivity of metals via direct nonequilibrium<i>ab initio</i>molecular dynamics. Physical Review B, 2016, 94, .	1.1	17
43	Anisotropic thermal and electrical transport properties induced high thermoelectric performance in an Ir₂Cl₂O₂ monolayer. Physical Chemistry Chemical Physics, 2022, 24, 11268-11277.	1.3	17
44	Surface Chemical Tuning of Phonon and Electron Transport in Free-Standing Silicon Nanowire Arrays. Nano Letters, 2016, 16, 6364-6370.	4.5	16
45	Unconventional magnetic anisotropy in one-dimensional Rashba system realized by adsorbing Gd atom on zigzag graphene nanoribbons. Nanoscale, 2017, 9, 11657-11666.	2.8	15
46	Bond saturation significantly enhances thermal energy transport in two-dimensional pentagonal materials. Nano Energy, 2018, 45, 1-9.	8.2	15
47	Hydrodynamically enhanced thermal transport due to strong interlayer interactions: A case study of strained bilayer graphene. Physical Review B, 2022, 105, .	1.1	15
48	Abnormal enhancement of thermal conductivity by planar structure: A comparative study of graphene-like materials. International Journal of Thermal Sciences, 2022, 174, 107438.	2.6	14
49	Half-negative Poissonâ€™s ratio in graphene+ with intrinsic Dirac nodal loop. Cell Reports Physical Science, 2022, 3, 100790.	2.8	14
50	Two-dimensional buckling structure induces the ultra-low thermal conductivity: a comparative study of the group GaX (X = N, P, As). Journal of Materials Chemistry C, 2022, 10, 1436-1444.	2.7	13
51	Enhancing thermal conductivity of silicone rubber composites by in-situ constructing SiC networks: A finite-element study based on first principles calculation. Nano Research, 2023, 16, 1430-1440.	5.8	13
52	Unprecedented mechanical response of the lattice thermal conductivity of auxetic carbon crystals. Carbon, 2017, 122, 374-380.	5.4	12
53	A C20 fullerene-based sheet with ultrahigh thermal conductivity. Nanoscale, 2018, 10, 6099-6104.	2.8	12
54	Unconventional thermal transport enhancement with large atom mass: a comparative study of 2D transition dichalcogenides. 2D Materials, 2018, 5, 015022.	2.0	12

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55	Experimental Studies of Thermal Conductivity of Three Biodiesel Compounds: Methyl Pentanoate, Methyl Octanoate, and Methyl Decanoate. Journal of Chemical & Engineering Data, 2022, 67, 45-53.	1.0	12
56	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
57	Rashba spin splitting and perpendicular magnetic anisotropy of Gd-adsorbed zigzag graphene nanoribbon modulated by edge states under external electric fields. Physical Review B, 2020, 101, .	1.1	11
58	Measurement of the thermal conductivity of the components of biodiesels: Methyl laurate and methyl myristate. Fluid Phase Equilibria, 2022, 556, 113409.	1.4	11
59	Ultralow lattice thermal conductivity and dramatically enhanced thermoelectric properties of monolayer InSe induced by an external electric field. Physical Chemistry Chemical Physics, 2021, 23, 13633-13646.	1.3	10
60	Novel optimization perspectives for thermoelectric properties based on Rashba spin splitting: a mini review. Nanoscale, 2021, 13, 18032-18043.	2.8	10
61	Computationally Guided Synthesis of High Performance Thermoelectric Materials: Defect Engineering in AgGaTe₂. Advanced Electronic Materials, 2021, 7, 2001262.	2.6	10
62	Dependence of phonon transport properties with stacking thickness in layered ZnO. Journal Physics D: Applied Physics, 2018, 51, 315303.	1.3	9
63	Different Effects of Mg and Si Doping on the Thermal Transport of Gallium Nitride. Frontiers in Materials, 2021, 8, .	1.2	9
64	Unique Arrangement of Atoms Leads to Low Thermal Conductivity: A Comparative Study of Monolayer Mg₂C. Journal of Physical Chemistry Letters, 2021, 12, 10353-10358.	2.1	7
65	The consistent behavior of negative Poisson's ratio with interlayer interactions. Materials Advances, 2022, 3, 4334-4341.	2.6	7
66	Energetics and magnetism of Co-doped GaN(0001) surfaces: A first-principles study. Journal of Applied Physics, 2014, 116, .	1.1	6
67	Thermal transport properties of monolayer phosphorene: a mini-review of theoretical studies. Frontiers in Energy, 2018, 12, 87-96.	1.2	6
68	Electrically-driven robust tuning of lattice thermal conductivity. Physical Chemistry Chemical Physics, 2022, 24, 17479-17484.	1.3	5
69	Quasi-bonding driven abnormal isotropic thermal transport in intrinsically anisotropic nanostructure: a case of study of a phosphorus nanotube array. Nanotechnology, 2020, 31, 095704.	1.3	3
70	Accessing negative Poissonâ€™s ratio of graphene by machine learning interatomic potentials. Nanotechnology, 2022, 33, 275710.	1.3	3
71	Multifunctional two-dimensional graphene-like boron nitride allotrope of g-B3N5: A competitor to g-BN?. Journal of Alloys and Compounds, 2022, 921, 165913.	2.8	3
72	Diverse Thermal Transport Properties of Two-Dimensional Materials: A Comparative Review. , 0, , .		2

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73	Ultra-high thermal conductivities of tetrahedral carbon allotropes with non-simple structures. Physical Chemistry Chemical Physics, 2021, 23, 24550-24556.	1.3	2
74	The stable behavior of low thermal conductivity in 1T-sandwich structure with different components. Journal of Applied Physics, 2022, 131, .	1.1	2
75	Uniform Strain-Dependent Thermal Conductivity of Pentagonal and Hexagonal Silicene. Frontiers in Materials, 2021, 8, .	1.2	1
76	Activated Lone-Pair Electrons Lead to Low Lattice Thermal Conductivity: A Case Study of Boron Arsenide. SSRN Electronic Journal, 0, , .	0.4	0
77	On the microscopic view of the low thermal conductivity of buckling two-dimensional materials from molecular dynamics. Chemical Physics Letters, 2021, 780, 138954.	1.2	0
78	Two-dimensional silicon. Series in Materials Science and Engineering, 2017, , 43-76.	0.1	0
79	Anisotropy of thermal transport in phosphorene: A comparative first-principles study using different exchange-correlation functional. Materials Advances, 0, , .	2.6	0
80	Introductory Chapter: Thermoelectricity â€“ Recent Advances, New Perspectives, and Applications. , 0, , .		0
81	N-doped graphene film prepared by rapid thermal shock for ultra-sensitive temperature reading. Applied Surface Science, 2022, 600, 154117.	3.1	0