## Guang-Zhao Qin

## List of Publications by Citations

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#	Paper	IF	Citations
68	Anisotropic intrinsic lattice thermal conductivity of phosphorene from first principles. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 4854-8	3.6	296
67	Hinge-like structure induced unusual properties of black phosphorus and new strategies to improve the thermoelectric performance. <i>Scientific Reports</i> , <b>2014</b> , 4, 6946	4.9	181
66	Thermal conductivity of silicene calculated using an optimized Stillinger-Weber potential. <i>Physical Review B</i> , <b>2014</b> , 89,	3.3	173
65	Diverse anisotropy of phonon transport in two-dimensional group IV-VI compounds: A comparative study. <i>Nanoscale</i> , <b>2016</b> , 8, 11306-19	7.7	170
64	Large tunability of lattice thermal conductivity of monolayer silicene via mechanical strain. <i>Physical Review B</i> , <b>2016</b> , 93,	3.3	132
63	Disparate Strain Dependent Thermal Conductivity of Two-dimensional Penta-Structures. <i>Nano Letters</i> , <b>2016</b> , 16, 3831-42	11.5	132
62	Tinselenidene: a Two-dimensional Auxetic Material with Ultralow Lattice Thermal Conductivity and Ultrahigh Hole Mobility. <i>Scientific Reports</i> , <b>2016</b> , 6, 19830	4.9	119
61	Orbitally driven low thermal conductivity of monolayer gallium nitride (GaN) with planar honeycomb structure: a comparative study. <i>Nanoscale</i> , <b>2017</b> , 9, 4295-4309	7.7	101
60	Resonant bonding driven giant phonon anharmonicity and low thermal conductivity of phosphorene. <i>Physical Review B</i> , <b>2016</b> , 94,	3.3	79
59	Anomalously temperature-dependent thermal conductivity of monolayer GaN with large deviations from the traditional 1/T law. <i>Physical Review B</i> , <b>2017</b> , 95,	3.3	71
58	Insight into the collective vibrational modes driving ultralow thermal conductivity of perovskite solar cells. <i>Physical Review B</i> , <b>2016</b> , 94,	3.3	41
57	External electric field driving the ultra-low thermal conductivity of silicene. <i>Nanoscale</i> , <b>2017</b> , 9, 7227-72	23 <del>/</del> 47	39
56	Low thermal conductivity of monolayer ZnO and its anomalous temperature dependence. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 12882-12889	3.6	37
55	Nontrivial contribution of FrBlich electron-phonon interaction to lattice thermal conductivity of wurtzite GaN. <i>Applied Physics Letters</i> , <b>2016</b> , 109, 242103	3.4	34
54	Thermal transport in novel carbon allotropes with sp2 or sp3 hybridization: An ab initio study. <i>Physical Review B</i> , <b>2017</b> , 95,	3.3	32
53	First-principles study of electronic, optical and thermal transport properties of group III <b>V</b> I monolayer MX (M = Ga, In; X = S, Se). <i>Journal of Applied Physics</i> , <b>2019</b> , 125, 245104	2.5	32
52	Lone-pair electrons induced anomalous enhancement of thermal transport in strained planar two-dimensional materials. <i>Nano Energy</i> , <b>2018</b> , 50, 425-430	17.1	32

## (2019-2020)

51	Thermal transport properties of GaN with biaxial strain and electron-phonon coupling. <i>Journal of Applied Physics</i> , <b>2020</b> , 127, 035102	2.5	29
50	Exploring T-carbon for energy applications. <i>Nanoscale</i> , <b>2019</b> , 11, 5798-5806	7.7	28
49	Negative Poisson artio in two-dimensional honeycomb structures. <i>Npj Computational Materials</i> , <b>2020</b> , 6,	10.9	27
48	Accelerating evaluation of converged lattice thermal conductivity. <i>Npj Computational Materials</i> , <b>2018</b> , 4,	10.9	26
47	Thermal Transport in Phosphorene. <i>Small</i> , <b>2018</b> , 14, e1702465	11	24
46	On the diversity in the thermal transport properties of graphene: A first-principles-benchmark study testing different exchange-correlation functionals. <i>Computational Materials Science</i> , <b>2018</b> , 151, 153-159	3.2	24
45	Origin of anisotropic negative Poisson's ratio in graphene. <i>Nanoscale</i> , <b>2018</b> , 10, 10365-10370	7.7	22
44	Metric for strong intrinsic fourth-order phonon anharmonicity. <i>Physical Review B</i> , <b>2017</b> , 95,	3.3	19
43	Lone-Pair Electrons Do Not Necessarily Lead to Low Lattice Thermal Conductivity: An Exception of Two-Dimensional Penta-CN. <i>Journal of Physical Chemistry Letters</i> , <b>2018</b> , 9, 2474-2483	6.4	17
42	Methodology for determining the electronic thermal conductivity of metals via direct nonequilibrium ab initio molecular dynamics. <i>Physical Review B</i> , <b>2016</b> , 94,	3.3	16
41	Behavior of aluminum adsorption and incorporation at GaN(0001) surface: First-principles study. <i>Journal of Applied Physics</i> , <b>2013</b> , 114, 194307	2.5	16
40	Surface Chemical Tuning of Phonon and Electron Transport in Free-Standing Silicon Nanowire Arrays. <i>Nano Letters</i> , <b>2016</b> , 16, 6364-6370	11.5	14
39	Giant effect of spinlattice coupling on the thermal transport in two-dimensional ferromagnetic CrI3. <i>Journal of Materials Chemistry C</i> , <b>2020</b> , 8, 3520-3526	7.1	13
38	Strain-modulated electronic and thermal transport properties of two-dimensional O-silica. <i>Nanotechnology</i> , <b>2016</b> , 27, 265706	3.4	13
37	Disparate strain response of the thermal transport properties of bilayer penta-graphene as compared to that of monolayer penta-graphene. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 15647-1	5855	12
36	Bond saturation significantly enhances thermal energy transport in two-dimensional pentagonal materials. <i>Nano Energy</i> , <b>2018</b> , 45, 1-9	17.1	12
35	Phonon transport in the ground state of two-dimensional silicon and germanium. <i>RSC Advances</i> , <b>2016</b> , 6, 69956-69965	3.7	12
34	Two-dimensional magnetic metal-organic frameworks with the Shastry-Sutherland lattice. <i>Chemical Science</i> , <b>2019</b> , 10, 10381-10387	9.4	11

33	Unconventional magnetic anisotropy in one-dimensional Rashba system realized by adsorbing Gd atom on zigzag graphene nanoribbons. <i>Nanoscale</i> , <b>2017</b> , 9, 11657-11666	7.7	9
32	Methodology Perspective of Computing Thermal Transport in Low-Dimensional Materials and Nanostructures: The Old and the New. <i>ACS Omega</i> , <b>2018</b> , 3, 3278-3284	3.9	8
31	Measurements and calculations of thermal conductivity for liquid n-octane and n-decane. <i>Fluid Phase Equilibria</i> , <b>2021</b> , 533, 112940	2.5	8
30	Unconventional thermal transport enhancement with large atom mass: a comparative study of 2D transition dichalcogenides. <i>2D Materials</i> , <b>2018</b> , 5, 015022	5.9	8
29	Efficient thermal conductivity modulation by manipulating interlayer interactions: A comparative study of bilayer graphene and graphite. <i>Journal of Applied Physics</i> , <b>2019</b> , 126, 125104	2.5	7
28	Unprecedented mechanical response of the lattice thermal conductivity of auxetic carbon crystals. <i>Carbon</i> , <b>2017</b> , 122, 374-380	10.4	7
27	Two-dimensional Al2I2Se2: A promising anisotropic thermoelectric material. <i>Journal of Alloys and Compounds</i> , <b>2021</b> , 876, 160191	5.7	7
26	A C fullerene-based sheet with ultrahigh thermal conductivity. <i>Nanoscale</i> , <b>2018</b> , 10, 6099-6104	7.7	6
25	Dependence of phonon transport properties with stacking thickness in layered ZnO. <i>Journal Physics D: Applied Physics</i> , <b>2018</b> , 51, 315303	3	6
24	Energetics and magnetism of Co-doped GaN(0001) surfaces: A first-principles study. <i>Journal of Applied Physics</i> , <b>2014</b> , 116, 224503	2.5	6
23	The exceptionally high thermal conductivity after 'alloying' two-dimensional gallium nitride (GaN) and aluminum nitride (AlN). <i>Nanotechnology</i> , <b>2021</b> , 32, 135401	3.4	5
22	Measurement and modeling of thermal conductivity for short chain methyl esters: Methyl butyrate and methyl caproate. <i>Journal of Chemical Thermodynamics</i> , <b>2021</b> , 159, 106486	2.9	5
21	Novel optimization perspectives for thermoelectric properties based on Rashba spin splitting: a mini review. <i>Nanoscale</i> , <b>2021</b> , 13, 18032-18043	7.7	4
20	Thermal conductivity measurements for long-chain n-alkanes at evaluated temperature and pressure: n-dodecane and n-tetradecane. <i>Journal of Chemical Thermodynamics</i> , <b>2021</b> , 162, 106566	2.9	4
19	Thermal conductivity of polydisperse hexagonal BN/polyimide composites: Iterative EMT model and machine learning based on first principles investigation. <i>Chemical Engineering Journal</i> , <b>2022</b> , 437, 135438	14.7	4
18	Rashba spin splitting and perpendicular magnetic anisotropy of Gd-adsorbed zigzag graphene nanoribbon modulated by edge states under external electric fields. <i>Physical Review B</i> , <b>2020</b> , 101,	3.3	3
17	Two-dimensional layered MSiN (M = Mo, W) as promising thermal management materials: a comparative study <i>Physical Chemistry Chemical Physics</i> , <b>2022</b> ,	3.6	3
16	Computationally Guided Synthesis of High Performance Thermoelectric Materials: Defect Engineering in AgGaTe2. <i>Advanced Electronic Materials</i> , <b>2021</b> , 7, 2001262	6.4	3

## LIST OF PUBLICATIONS

15	Thermal transport properties of monolayer phosphorene: a mini-review of theoretical studies. <i>Frontiers in Energy</i> , <b>2018</b> , 12, 87-96	2.6	2
14	Measurement of the thermal conductivity of the components of biodiesels: Methyl laurate and methyl myristate. <i>Fluid Phase Equilibria</i> , <b>2022</b> , 556, 113409	2.5	2
13	Experimental Studies of Thermal Conductivity of Three Biodiesel Compounds: Methyl Pentanoate, Methyl Octanoate, and Methyl Decanoate. <i>Journal of Chemical &amp; Engineering Data</i> , <b>2022</b> , 67, 45-53	2.8	2
12	Unique Arrangement of Atoms Leads to Low Thermal Conductivity: A Comparative Study of Monolayer MgC. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 10353-10358	6.4	2
11	Quasi-bonding driven abnormal isotropic thermal transport in intrinsically anisotropic nanostructure: a case of study of a phosphorus nanotube array. <i>Nanotechnology</i> , <b>2020</b> , 31, 095704	3.4	2
10	Intrinsically low lattice thermal conductivity of monolayer hexagonal aluminum nitride (h-AlN) from first-principles: A comparative study with graphene. <i>International Journal of Thermal Sciences</i> , <b>2021</b> , 162, 106772	4.1	2
9	Diverse Thermal Transport Properties of Two-Dimensional Materials: A Comparative Review 2016,		2
8	Ultralow lattice thermal conductivity and dramatically enhanced thermoelectric properties of monolayer InSe induced by an external electric field. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 1363	ı3÷136	46
7	Ultra-high thermal conductivities of tetrahedral carbon allotropes with non-simple structures. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 24550-24556	3.6	1
6	Half-negative Poisson ratio in graphene+ with intrinsic Dirac nodal loop. <i>Cell Reports Physical Science</i> , <b>2022</b> , 3, 100790	6.1	1
5	The stable behavior of low thermal conductivity in 1T-sandwich structure with different components. <i>Journal of Applied Physics</i> , <b>2022</b> , 131, 185702	2.5	1
4	Abnormal enhancement of thermal conductivity by planar structure: A comparative study of graphene-like materials. <i>International Journal of Thermal Sciences</i> , <b>2022</b> , 174, 107438	4.1	O
3	Two-dimensional silicon. Series in Materials Science and Engineering, 2017, 43-76		
2	On the microscopic view of the low thermal conductivity of buckling two-dimensional materials from molecular dynamics. <i>Chemical Physics Letters</i> , <b>2021</b> , 780, 138954	2.5	

1 Introductory Chapter: Thermoelectricity [Recent Advances, New Perspectives, and Applications