

CITATION REPORT

List of articles citing

Phonon transport in single-layer transition metal dichalcogenides: A first-principles study

DOI: 10.1063/1.4896685

Applied Physics Letters, 2014, 105, 131903.

Source: <https://exaly.com/paper-pdf/58191899/citation-report.pdf>

Version: 2024-04-27

This report has been generated based on the citations recorded by exaly.com for the above article. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

#	Paper	IF	Citations
277	Measurement of the anisotropic thermal conductivity of molybdenum disulfide by the time-resolved magneto-optic Kerr effect. 2014 , 116, 233107		173
276	Competing mechanism driving diverse pressure dependence of thermal conductivity of XTe (X=Hg,Cd, and Zn). <i>Physical Review B</i> , 2015 , 92,	3.3	51
275	First-Principles Determination of Ultralow Thermal Conductivity of monolayer WSe ₂ . 2015 , 5, 15070		61
274	Optical Limiting and Theoretical Modelling of Layered Transition Metal Dichalcogenide Nanosheets. 2015 , 5, 14646		174
273	Unusual isotope effect on thermal transport of single layer molybdenum disulphide. <i>Applied Physics Letters</i> , 2015 , 107, 191907	3.4	30
272	Thermal conductivity of biaxial-strained MoS ₂ : sensitive strain dependence and size dependent reduction rate. 2015 , 26, 465707		40
271	Cross-plane phonon transport properties of molybdenum disulphide. 2015 , 48, 465303		4
270	Two-dimensional materials and their prospects in transistor electronics. <i>Nanoscale</i> , 2015 , 7, 8261-83	7.7	415
269	Computational Search for Two-Dimensional MX ₂ Semiconductors with Possible High Electron Mobility at Room Temperature. 2016 , 9,		90
268	Towards intrinsic phonon transport in single-layer MoS ₂ . 2016 , 528, 504-511		53
267	Low lattice thermal conductivity of stanene. 2016 , 6, 20225		132
266	Ballistic thermal transport in monolayer transition-metal dichalcogenides: Role of atomic mass. <i>Applied Physics Letters</i> , 2016 , 108, 082102	3.4	12
265	Beyond Perturbation: Role of Vacancy-Induced Localized Phonon States in Thermal Transport of Monolayer MoS ₂ . <i>Journal of Physical Chemistry C</i> , 2016 , 120, 29324-29331	3.8	26
264	Phonon transport properties of two-dimensional group-IV materials from ab initio calculations. <i>Physical Review B</i> , 2016 , 94,	3.3	114
263	Layer thickness-dependent phonon properties and thermal conductivity of MoS ₂ . 2016 , 119, 085106		89
262	Phonons in bulk and monolayer HfS ₂ and possibility of phonon-mediated superconductivity: A first-principles study. <i>Solid State Communications</i> , 2016 , 237-238, 14-18	1.6	17
261	First-principles study of thermal properties of borophene. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 14927-32	3.6	85

260	Strain-induced enhancement in the thermoelectric performance of a ZrS ₂ monolayer. 2016 , 4, 4538-4545		130
259	Hydrogenation of Penta-Graphene Leads to Unexpected Large Improvement in Thermal Conductivity. 2016 , 16, 3925-35		109
258	Thermal conductivity of MoS ₂ polycrystalline nanomembranes. 2016 , 3, 035016		32
257	High-Throughput Computational Screening of Electrical and Phonon Properties of Two-Dimensional Transition Metal Dichalcogenides. 2016 , 68, 2666-2672		4
256	Enhanced thermoelectric power in two-dimensional transition metal dichalcogenide monolayers. <i>Physical Review B</i> , 2016 , 94,	3-3	45
255	Phonon transport in single-layer Mo _{1-x} W _x S ₂ alloy embedded with WS ₂ nanodomains. <i>Physical Review B</i> , 2016 , 94,	3-3	15
254	Thermal transport in van der Waals solids from first-principles calculations. <i>Physical Review B</i> , 2016 , 94,	3-3	67
253	Strong anisotropic thermal conductivity of monolayer WTe ₂ . 2016 , 3, 045010		31
252	Thermal Conductivity of Wurtzite Zinc-Oxide from First-Principles Lattice Dynamics--a Comparative Study with Gallium Nitride. 2016 , 6, 22504		85
251	A theoretical prediction of super high-performance thermoelectric materials based on MoS ₂ /WS ₂ hybrid nanoribbons. 2016 , 6, 21639		50
250	Thermal Conductivity of Monolayer MoSe ₂ and MoS ₂ . <i>Journal of Physical Chemistry C</i> , 2016 , 120, 26067-26075	3-6	69
249	Comparative study of thermal properties of group-VA monolayers with buckled and puckered honeycomb structures. <i>Physical Review B</i> , 2016 , 94,	3-3	39
248	Tuning thermal conductivity in molybdenum disulfide by electrochemical intercalation. 2016 , 7, 13211		101
247	Electronic and magnetic properties of 1T-HfS ₂ by doping transition-metal atoms. <i>Applied Surface Science</i> , 2016 , 383, 151-158	6-7	27
246	Anisotropic thermal transport in Weyl semimetal TaAs: a first principles calculation. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 16709-14	3-6	26
245	Thermal conductivity of monolayer MoS ₂ , MoSe ₂ , and WS ₂ : interplay of mass effect, interatomic bonding and anharmonicity. 2016 , 6, 5767-5773		202
244	Thermal transport properties of MoS ₂ and MoSe ₂ monolayers. 2016 , 27, 055703		66
243	First-principles calculations of thermal, electrical, and thermoelectric transport properties of semiconductors. 2016 , 31, 043001		42

- 242 Thermal Properties of Two Dimensional Layered Materials. *Advanced Functional Materials*, **2017**, 27, 1604134 96
- 241 Titanium Trisulfide Monolayer as a Potential Thermoelectric Material: A First-Principles-Based Boltzmann Transport Study. **2017**, 9, 2509-2515 60
- 240 The impact of hydrogenation on the thermal transport of silicene. **2017**, 4, 025002 15
- 239 Excellent Thermoelectric Properties in monolayer WSe Nanoribbons due to Ultralow Phonon Thermal Conductivity. **2017**, 7, 41418 26
- 238 Structural, electrical, phonon, and optical properties of Ti- and V-doped two-dimensional MoS₂. **2017**, 674, 157-163 23
- 237 The conflicting role of buckled structure in phonon transport of 2D group-IV and group-V materials. *Nanoscale*, **2017**, 9, 7397-7407 7.7 96
- 236 Spin heat capacity of monolayer and AB-stacked bilayer MoS₂ in the presence of exchange magnetic field. **2017**, 104, 331-340 5
- 235 Strain effects on phonon transport in antimonene investigated using a first-principles study. *Physical Chemistry Chemical Physics*, **2017**, 19, 14520-14526 3.6 32
- 234 On the influence of junction structures on the mechanical and thermal properties of carbon honeycombs. **2017**, 119, 278-286 44
- 233 Thermal Light Emission from Monolayer MoS. *Advanced Materials*, **2017**, 29, 1701304 24 32
- 232 The Effective Mass of Dirac Fermions and Spin-Dependent Thermodynamic Properties of Monolayer Ferromagnetic MoS₂ in the Presence of Rashba Spin-Orbit Coupling. **2017**, 30, 3137-3141 2
- 231 Exotic thermoelectric behavior in nitrogenated holey graphene. **2017**, 7, 25803-25810 19
- 230 A systematic investigation of thermal conductivities of transition metal dichalcogenides. **2017**, 108, 417-422 28
- 229 Magnetic doping in two-dimensional transition-metal dichalcogenide zirconium diselenide. *Journal of Alloys and Compounds*, **2017**, 698, 611-616 5.7 17
- 228 How to characterize thermal transport capability of 2D materials fairly? Sheet thermal conductance and the choice of thickness. **2017**, 669, 233-237 75
- 227 Induced magnetism in transition metal-doped 1T-ZrS₂. *Journal of Alloys and Compounds*, **2017**, 695, 20485-2053 19
- 226 Record Low Thermal Conductivity of Polycrystalline MoS Films: Tuning the Thermal Conductivity by Grain Orientation. **2017**, 9, 37905-37911 26
- 225 Thermal conductivity modeling of hybrid organic-inorganic crystals and superlattices. **2017**, 41, 394-407 21

224	Effects of Defects on the Temperature-Dependent Thermal Conductivity of Suspended Monolayer Molybdenum Disulfide Grown by Chemical Vapor Deposition. <i>Advanced Functional Materials</i> , 2017 , 27, 1704357	15.6	31
223	Phonon spectra, electronic, and thermodynamic properties of WS nanotubes. 2017 , 38, 2581-2593		21
222	Anisotropic lattice thermal conductivity in three-fold degeneracy topological semimetal MoP: a first-principles study. <i>Journal of Physics Condensed Matter</i> , 2017 , 29, 435704	1.8	12
221	Probing Anisotropic Thermal Conductivity of Transition Metal Dichalcogenides MX (M = Mo, W and X = S, Se) using Time-Domain Thermoreflectance. <i>Advanced Materials</i> , 2017 , 29, 1701068	24	107
220	Effect of the accuracy of interatomic force constants on the prediction of lattice thermal conductivity. 2017 , 138, 368-376		9
219	A first-principles study of phonon transport properties of monolayer MoSe ₂ . 2017 ,		
218	Convergence of separate orbits for enhanced thermoelectric performance of layered ZrS ₂ . 2017 , 19, 073036		17
217	Anharmonic, dimensionality and size effects in phonon transport. <i>Journal of Physics Condensed Matter</i> , 2017 , 29, 505703	1.8	10
216	Thermoelectric properties of two-dimensional transition metal dichalcogenides. 2017 , 5, 7684-7698		125
215	Ultra low lattice thermal conductivity and high carrier mobility of monolayer SnS and SnSe: a first principles study. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 20677-20683	3.6	110
214	Thermoelectric properties of SnSe monolayer. <i>Journal of Physics Condensed Matter</i> , 2017 , 29, 015001	1.8	62
213	First-Principles Calculations of Thermoelectric Properties of IV-VI Chalcogenides 2D Materials. 2017 , 3,		17
212	Parameterization of Stillinger-Weber Potential for Two- Dimensional Atomic Crystals. 2017 ,		22
211	Ultrahigh lattice thermal conductivity in topological semimetal TaN caused by a large acoustic-optical gap. <i>Journal of Physics Condensed Matter</i> , 2018 , 30, 105701	1.8	5
210	Phonon transport in Janus monolayer MoSSe: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 7236-7242	3.6	89
209	Intrinsic electronic transport and thermoelectric power factor in n-type doped monolayer MoS ₂ . 2018 , 20, 043009		17
208	Influence of defects and doping on phonon transport properties of monolayer MoSe ₂ . 2018 , 5, 031008		14
207	Review of thermal transport and electronic properties of borophene. 2018 , 27, 036303		18

206	Control of thermal conductivity with species mass in transition-metal dichalcogenides. 2018 , 123, 135703		5
205	Density functional theory study of inter-layer coupling in bulk tin selenide. 2018 , 695, 200-204		18
204	Monolayer and bilayer polyaniline CN: two-dimensional semiconductors with high thermal conductivity. <i>Nanoscale</i> , 2018 , 10, 4301-4310	7.7	72
203	Reduced Thermal Transport in the Graphene/MoS/Graphene Heterostructure: A Comparison with Freestanding Monolayers. 2018 , 34, 3326-3335		13
202	Strongly bound excitons in monolayer PtS ₂ and PtSe ₂ . <i>Applied Physics Letters</i> , 2018 , 112, 043101	3.4	47
201	Hidden spin polarization in the 1 T -phase layered transition-metal dichalcogenides MX ₂ (M = Zr, Hf; X = S, Se, Te). 2018 , 63, 85-91		16
200	Bond saturation significantly enhances thermal energy transport in two-dimensional pentagonal materials. 2018 , 45, 1-9		12
199	Effect of Metal Doping and Vacancies on the Thermal Conductivity of Monolayer Molybdenum Diselenide. 2018 , 10, 4921-4928		19
198	Unusually low thermal conductivity of atomically thin 2D tellurium. <i>Nanoscale</i> , 2018 , 10, 12997-13003	7.7	83
197	Soft phonon modes driven huge difference on lattice thermal conductivity between topological semimetal WC and WN. 2018 , 148, 144706		7
196	Thermal properties of transition-metal dichalcogenide. 2018 , 27, 034402		8
195	Anisotropic thermal conductivity in carbon honeycomb. <i>Journal of Physics Condensed Matter</i> , 2018 , 30, 155702	1.8	10
194	Origin of ultra-low lattice thermal conductivity in Cs ₂ BiAgX ₆ (X=Cl, Br) and its impact on thermoelectric performance. <i>Journal of Alloys and Compounds</i> , 2018 , 748, 63-72	5.7	38
193	Engineering of charge carriers via a two-dimensional heterostructure to enhance the thermoelectric figure of merit. <i>Nanoscale</i> , 2018 , 10, 7077-7084	7.7	44
192	Validation of inter-atomic potential for WS ₂ and WSe ₂ crystals through assessment of thermal transport properties. 2018 , 144, 92-98		23
191	Strain-induced enhancement of thermoelectric performance of TlS monolayer based on first-principles phonon and electron band structures. 2018 , 29, 015204		31
190	Colloquium: Phononic thermal properties of two-dimensional materials. 2018 , 90,		141
189	Nonmonotonic thickness-dependence of in-plane thermal conductivity of few-layered MoS ₂ : 2.4 to 37.8 nm. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 25752-25761	3.6	28

188	Two-dimensional MoS ₂ -MoSe ₂ lateral superlattice with minimized lattice thermal conductivity. 2018 , 124, 165101		15
187	Comparison of vibrational and thermodynamic properties of MoS ₂ and WS ₂ nanotubes: first principles study. 2018 , 5, 115028		6
186	A first-principles study of the effects of electron-phonon coupling on the thermoelectric properties: a case study of the SiGe compound. 2018 , 6, 12125-12131		20
185	Enhanced electronic and optical properties of three TMD heterobilayers. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 16604-16614	3.6	15
184	Localized interlayer complexes in heterobilayer transition metal dichalcogenides. <i>Physical Review B</i> , 2018 , 97,	3.3	18
183	Versatile mechanical properties of novel g-SiC monolayers from graphene to silicene: a first-principles study. 2018 , 29, 315701		16
182	Hybrid k tight-binding model for subbands and infrared intersubband optics in few-layer films of transition-metal dichalcogenides: MoS ₂ , MoSe ₂ , WS ₂ , and WSe ₂ . <i>Physical Review B</i> , 2018 , 98,	3.3	18
181	Thermal conductivity of hexagonal Si, Ge, and Si _{1-x} Ge _x alloys from first-principles. 2018 , 123, 185104		8
180	Nonmonotonic strain dependence of lattice thermal conductivity in monolayer SiC: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 22038-22046	3.6	17
179	Enhanced thermoelectric performance of two dimensional MS ₂ (M = Mo, W) through phase engineering. 2018 , 4, 329-337		11
178	Phonon band gaps in the IV-VI monochalcogenides. <i>Physical Review B</i> , 2019 , 100,	3.3	11
177	Phonon wind and drag of excitons in monolayer semiconductors. <i>Physical Review B</i> , 2019 , 100,	3.3	24
176	Temperature profiles and thermal conductivities of nanostructured transition metal dichalcogenides. 2019 , 140, 579-586		3
175	Systematic investigations of the electron, phonon and elastic properties of monolayer MC (M = V, Nb, Ta) by first-principles calculations. <i>Journal of Physics Condensed Matter</i> , 2019 , 31, 405703	1.8	8
174	Temperature-dependent phonon spectrum of transition metal dichalcogenides calculated from the spectral energy density: Lattice thermal conductivity as an application. <i>Physical Review B</i> , 2019 , 100,	3.3	11
173	Dominant ZA phonons and thermal carriers in HfS ₂ . 2019 , 126, 164302		4
172	Thermoelectric Performance of Two-Dimensional AlX (X = S, Se, Te): A First-Principles-Based Transport Study. <i>ACS Omega</i> , 2019 , 4, 17773-17781	3.9	27
171	Thermal conductivity modeling using machine learning potentials: application to crystalline and amorphous silicon. 2019 , 10, 100140		23

170	Born effective charge removed anomalous temperature dependence of lattice thermal conductivity in monolayer GeC. <i>Journal of Physics Condensed Matter</i> , 2019 , 31, 125701	1.8	3
169	Thermal conductivity of MoS ₂ /MoSe ₂ heterostructures: The role of lattice mismatch, interlayer rotation and species intermixing. 2019 , 143, 118583		10
168	Field enhanced in-plane homostructure in a pure MoSe ₂ phototransistor for the efficient separation of photo-excited carriers. 2019 , 7, 1182-1187		5
167	Electronic structure, optical properties, and phonon transport in Janus monolayer PtSSe via first-principles study. 2019 , 99, 1025-1040		37
166	Effects of tensile strain and finite size on thermal conductivity in monolayer WSe. <i>Physical Chemistry Chemical Physics</i> , 2018 , 21, 468-477	3.6	36
165	The magnetism of 1T-MX (M = Zr, Hf; X = S, Se) monolayers by hole doping.. 2019 , 9, 13561-13566		10
164	Origins of promising thermoelectric performance in quaternary selenide BaAg ₂ SnSe ₄ . 2019 , 12, 071006		3
163	Theoretical Investigation of Metal-Shrouded Tl ₂ O Monolayers: Pudding-Mold-Type Band Structure and Thermoelectric Performance. 2019 , 2, 4061-4066		15
162	Energy dissipation in van der Waals 2D devices. 2019 , 6, 032005		13
161	Ultra-Long Lifetimes of Single Quantum Emitters in Monolayer WSe ₂ /hBN Heterostructures. 2019 , 2, 1900022		8
160	Ultralow Lattice Thermal Conductivity and Thermoelectric Properties of Monolayer Tl ₂ O. 2019 , 2, 3004-3008		29
159	Thermal conductivity of single-layer MoS ₂ (1-x)Se _{2x} alloys from molecular dynamics simulations with a machine-learning-based interatomic potential. 2019 , 165, 74-81		27
158	Thermal conductivity and phonon hydrodynamics in transition metal dichalcogenides from first-principles. 2019 , 6, 035002		25
157	Electronic and vibrational properties of van der Waals heterostructures of vertically stacked few-layer atomically thin MoS ₂ and BP. 2019 , 19, 383-392		7
156	Thermal conductivity of MoS ₂ monolayers from molecular dynamics simulations. 2019 , 9, 035042		13
155	Intrinsic Thermal conductivities of monolayer transition metal dichalcogenides MX (M = Mo, W; X = S, Se, Te). 2019 , 9, 4571		26
154	First-principles study of elastic, thermal and optical properties of a metal-shrouded two-dimensional semiconductor Tl ₂ O. <i>Solid State Communications</i> , 2019 , 293, 40-47	1.6	4
153	Energy Dissipation in Black Phosphorus Heterostructured Devices. 2019 , 6, 1801528		9

152	Frequency-domain energy transport state-resolved Raman for measuring the thermal conductivity of suspended nm-thick MoSe ₂ . 2019 , 133, 1074-1085		33
151	Ultralow thermal conductivity of turbostratically disordered MoSe ultra-thin films and implications for heterostructures. 2019 , 30, 285401		16
150	Theoretical investigation of electronic structure and thermoelectric properties of MX ₂ (M=Zr, Hf; X=S, Se) van der Waals heterostructures. 2019 , 126, 304-309		19
149	Recent progress on graphene-analogous 2D nanomaterials: Properties, modeling and applications. 2019 , 100, 99-169		160
148	Thermal Transport in 2D Semiconductors: Considerations for Device Applications. <i>Advanced Functional Materials</i> , 2020 , 30, 1903929	15.6	41
147	First-Principles Calculations of Phonons and Thermodynamic Properties of Zr(Hf)S -Based Nanotubes. 2020 , 41, 759-768		2
146	2D Materials for Large-Area Flexible Thermoelectric Devices. <i>Advanced Energy Materials</i> , 2020 , 10, 19028428	8.428	72
145	First-principles study of phonon thermal transport in III-V group graphenelike materials. 2020 , 38, 062202		1
144	Strong electron-phonon interaction induced significant reduction in lattice thermal conductivities for single-layer MoS ₂ and PtSSe. 2020 , 15, 100277		8
143	Thermal transport properties of novel two-dimensional CSe. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 17833-17841	3.6	4
142	Effect of biaxial strain on thermal transport in WS ₂ monolayer from first principles calculations. 2020 , 124, 114312		9
141	Borophene: New Sensation in Flatland. <i>Advanced Materials</i> , 2020 , 32, e2000531	24	41
140	The Effect of Janus Asymmetry on Thermal Transport in SnSSe. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 17476-17484	3.8	9
139	Anomalous layer thickness dependent thermal conductivity of Td-WTe ₂ through first-principles calculation. 2020 , 384, 126751		3
138	Structural dynamics of incommensurate charge-density waves tracked by ultrafast low-energy electron diffraction. 2020 , 7, 034304		11
137	Strain-Induced Ultrahigh Electron Mobility and Thermoelectric Figure of Merit in Monolayer HfTe. 2020 , 12, 43901-43910		10
136	High Thermoelectric Performance in Two-Dimensional Janus Monolayer Material WS-X (X = Se and Te). 2020 , 12, 46212-46219		35
135	Promising high-temperature thermoelectric response of bismuth oxybromide. 2020 , 19, 103584		9

134	Thermal Transport in Two-Dimensional Heterostructures. 2020 , 7,		4
133	Experimental Study on Thermal Conductivity and Rectification in Suspended Monolayer MoS. 2020 , 12, 28306-28312		9
132	Dynamically reconfigurable electronic and phononic properties in intercalated HfS ₂ . 2020 , 39, 110-117		2
131	Ultra-low thermal conductivity and super-slow hot-carrier thermalization induced by a huge phononic gap in multifunctional nanoscale boron pnictides. 2020 , 124, 114222		13
130	Tunable thermal conductivity of single layer MoS ₂ nanoribbons: an equilibrium molecular dynamics study. 2020 , 19, 957-965		2
129	Role of Optical Phonons in Bulk Molybdenum Diselenide Thermal Properties Probed by Advanced Raman Spectroscopy. 2020 , 257, 2000251		2
128	Ultra-low lattice thermal conductivity and giant phonon-electric field coupling in hafnium dichalcogenide monolayers. <i>Journal of Physics Condensed Matter</i> , 2020 , 32, 315301	1.8	11
127	Thermodynamic and thermoelectric properties of CoFeYGe (Y = Ti, Cr) quaternary Heusler alloys: first principle calculations. <i>Journal of Physics Condensed Matter</i> , 2020 , 32, 075402	1.8	14
126	Size-dependent phononic thermal transport in low-dimensional nanomaterials. 2020 , 860, 1-26		110
125	In-Plane and Interfacial Thermal Conduction of Two-Dimensional Transition-Metal Dichalcogenides. 2020 , 13,		19
124	Phonon Thermal Properties of Heterobilayers with a Molecular Dynamics Study. 2020 , 41, 1		3
123	Current Rerouting Improves Heat Removal in Few-Layer WSe Devices. 2020 , 12, 14323-14330		6
122	A thin film efficient pn-junction thermoelectric device fabricated by self-align shadow mask. 2020 , 10, 1067		13
121	Recent Progress of Two-Dimensional Thermoelectric Materials. 2020 , 12, 36		98
120	Thermal transport of chalcogenides. 2020 , 339-370		1
119	HfS/MoTe vdW heterostructure: bandstructure and strain engineering based on first-principles calculation.. 2020 , 10, 2615-2623		9
118	Thermoelectric properties of Janus MXY (M = Pd, Pt; X, Y = S, Se, Te) transition-metal dichalcogenide monolayers from first principles. 2020 , 127, 035101		36
117	Strain tunable pudding-mold-type band structure and thermoelectric properties of SnP ₃ monolayer. 2020 , 127, 155103		5

116	Prediction of Nanoscale Friction for Two-Dimensional Materials Using a Machine Learning Approach. 2020 , 68, 1		15
115	Low-temperature thermoelectric behavior and impressive optoelectronic properties of two-dimensional XI_2 ($X = Sn, Si$): A first principle study. 2021 , 186, 109977		11
114	Reduced thermal conductivity of supported and encased monolayer and bilayer MoS ₂ . 2021 , 8, 011001		10
113	Thermoelectric and lattice dynamics properties of layered MX ($M = Sn, Pb$; $X = S, Te$) compounds. <i>Applied Surface Science</i> , 2021 , 538, 147911	6.7	10
112	The first-principles and BTE investigation of phonon transport in 1T-TiSe. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 1627-1638	3.6	5
111	First-principles studies of MoF ₆ absorption on hydroxylated and non-hydroxylated metal oxide surfaces and implications for atomic layer deposition of MoS ₂ . <i>Applied Surface Science</i> , 2021 , 541, 148461	6.7	2
110	Improved thermoelectric properties of WS ₂ -WSe ₂ phononic crystals: insights from first-principles calculations. <i>Nanoscale</i> , 2021 , 13, 7176-7192	7.7	7
109	The impact of electron-phonon coupling on the figure of merit of NbSiTe and NbGeTe ternary monolayers. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 15613-15619	3.6	2
108	Anomalous Low Thermal Conductivity of Atomically Thin InSe Probed by Scanning Thermal Microscopy. <i>Advanced Functional Materials</i> , 2021 , 31, 2008967	15.6	4
107	The exceptionally high thermal conductivity after alloying two-dimensional gallium nitride (GaN) and aluminum nitride (AlN). 2021 , 32, 135401		5
106	Phase diagram and superlattice structures of monolayer phosphorus carbide (P_xC_{1-x}). <i>Physical Review Materials</i> , 2021 , 5,	3.2	1
105	INTRODUCTION TO TWO-DIMENSIONAL MATERIALS. 2021 , 28, 2140005		6
104	First-principles analysis of phonon thermal transport properties of two-dimensional WS ₂ /WSe ₂ heterostructures*. 2021 , 30, 034401		5
103	Sulfide Perovskites for Thermoelectricity. 2021 , 13, 14189-14197		4
102	Experimental and Computational Investigation of Layer-Dependent Thermal Conductivities and Interfacial Thermal Conductance of One- to Three-Layer WSe ₂ . 2021 , 13, 13063-13071		9
101	Enhanced thermoelectric properties in two-dimensional monolayer Si ₂ BN by adsorbing halogen atoms*. 2021 , 30, 037304		1
100	2D Nb ₂ SiTe ₄ and Nb ₂ GeTe ₄ : promising thermoelectric figure of merit and gate-tunable thermoelectric performance. 2021 ,		2
99	Origins of Minimized Lattice Thermal Conductivity and Enhanced Thermoelectric Performance in WS ₂ /WSe ₂ Lateral Superlattice. <i>ACS Omega</i> , 2021 , 6, 7879-7886	3.9	9

98	Exceptional piezoelectricity, high thermal conductivity and stiffness and promising photocatalysis in two-dimensional MoSi ₂ N ₄ family confirmed by first-principles. 2021 , 82, 105716		70
97	Experimental study on thermal conductivity and rectification of monolayer and multilayer MoS ₂ . 2021 , 170, 121013		5
96	Ultralow Thermal Conductivity in Two-Dimensional MoO ₃ . 2021 , 21, 4351-4356		16
95	First-principles study of structural, electronic, and thermal conductivity properties of monolayer SrFBr. 2021 , 153, 109956		1
94	The effect of atomistic substitution on thermal transport in large phonon bandgap GaN. 2021 , 60, 071003		1
93	Thermal conductance of nanostructured interfaces from Monte Carlo simulations with ab initio-based phonon properties. 2021 , 129, 215105		2
92	Understanding the anisotropic phonon thermal transport through 2D Biligraphene. 2021 , 179, 523-530		
91	Multi-objective parametrization of interatomic potentials for large deformation pathways and fracture of two-dimensional materials. 2021 , 7,		0
90	The effect of finite-temperature and anharmonic lattice dynamics on the thermal conductivity of ZrSmonolayer: self-consistent phonon calculations. <i>Journal of Physics Condensed Matter</i> , 2021 , 33,	1.8	1
89	Novel thermoelectric performance of 2D 1T- SeTe and SeTewith ultralow lattice thermal conductivity but high carrier mobility. 2021 , 32,		4
88	Different Effects of Mg and Si Doping on the Thermal Transport of Gallium Nitride. 2021 , 8,		3
87	Effects of the vacancy and doping on the electronic and magnetic characteristics of ZrSe ₂ monolayer: A first-principles investigation. 2021 , 732, 138790		1
86	n-Type thermoelectric properties of a hexagonal SiGe polymorph superior to a cubic SiGe. <i>Journal of Alloys and Compounds</i> , 2021 , 874, 160007	5.7	0
85	Thermal transport property of novel two-dimensional nitride phosphorus: An ab initio study. <i>Applied Surface Science</i> , 2021 , 559, 149463	6.7	3
84	Low thermal conductivity: fundamentals and theoretical aspects in thermoelectric applications. 2021 , 21, 100744		13
83	High and Anomalous Thermal Conductivity in Monolayer MSiZ Semiconductors. 2021 , 13, 45907-45915		7
82	High electrical transport performance and ultralow thermal conductivity realized in Ga doped single-layer octagon-square nitrogene. <i>Applied Surface Science</i> , 2021 , 563, 150244	6.7	
81	The in-plane structure domain size of nm-thick MoSe uncovered by low-momentum phonon scattering. <i>Nanoscale</i> , 2021 , 13, 7723-7734	7.7	3

80	Lower lattice thermal conductivity in SbAs than As or Sb monolayers: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 31982-31988	3.6	32
79	Role of defects and phonons in bandgap dynamics of monolayer WS ₂ at high carrier densities. 2020 , 4, 015005		3
78	Defect-limited thermal conductivity in MoS ₂ . <i>Physical Review Materials</i> , 2020 , 4,	3.2	7
77	Tuning structural and electronic properties of two-dimensional aluminum monochalcogenides: Prediction of Janus Al ₂ XX' (X/X':O,S,Se,Te) monolayers. <i>Physical Review Materials</i> , 2020 , 4,	3.2	17
76	Effects of alloying on in-plane thermal conductivity and thermal boundary conductance in transition metal dichalcogenide monolayers. <i>Physical Review Materials</i> , 2020 , 4,	3.2	2
75	Optical Patterning of Two-Dimensional Materials. <i>Research</i> , 2020 , 2020, 6581250	7.8	17
74	Recent progresses of thermal conduction in two-dimensional materials. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2020 , 69, 196602	0.6	1
73	First-principles study on structural, vibrational, elastic, piezoelectric, and electronic properties of the Janus BiXY (X=S,Se,Te and Y=F,Cl,Br,I) monolayers. <i>Physical Review Materials</i> , 2021 , 5,	3.2	4
72	Improved Thermoelectric Performance of Monolayer HfS by Strain Engineering. <i>ACS Omega</i> , 2021 , 6, 29820-29829	3.9	3
71	Electron-phonon coupling contribution on the optical absorption and the dynamic of exciton-polaron in monolayer Transition Metal Dichalcogenides. <i>Optical and Quantum Electronics</i> , 2021 , 53, 1	2.4	0
70	First-Principles Study of the Physical Properties of Novel Polytypes of Gallium Phosphide. <i>Crystal Growth and Design</i> ,	3.5	4
69	Atomic-level defect modulation and characterization methods in 2D materials. <i>APL Materials</i> , 2021 , 9, 100902	5.7	5
68	Large exciton binding energy, superior mechanical flexibility, and ultra-low lattice thermal conductivity in Bilmonolayer. <i>Journal of Physics Condensed Matter</i> , 2021 , 34,	1.8	
67	The role of mid-gap phonon modes in thermal transport of transition metal dichalcogenides. <i>Journal of Physics Condensed Matter</i> , 2020 , 32, 025306	1.8	2
66	Chalcogenides. <i>Nanoscience and Technology</i> , 2020 , 631-833	0.6	
65	Strong interlayer coupling in two-dimensional PbSe with high thermoelectric performance. <i>Journal of Physics Condensed Matter</i> , 2021 , 33,	1.8	3
64	Low thermal conductivity and interface thermal conductance in SnS ₂ . <i>Physical Review B</i> , 2021 , 104,	3.3	0
63	Thermoelectric properties of Janus AsSBr monolayer from first-principles study. <i>Solid State Communications</i> , 2021 , 114612	1.6	1

62	Ultralow lattice thermal conductivity at room temperature in 2D KCuSe from first-principles calculations.. <i>Physical Chemistry Chemical Physics</i> , 2022 ,	3.6	0
61	Grain boundary and misorientation angle-dependent thermal transport in single-layer MoS ₂ .. <i>Nanoscale</i> , 2022 ,	7.7	1
60	Abnormal enhancement of thermal conductivity by planar structure: A comparative study of graphene-like materials. <i>International Journal of Thermal Sciences</i> , 2022 , 174, 107438	4.1	0
59	Thermal Conductivities and Interfacial Thermal Conductance of 2D WSe ₂ . 2020 ,		1
58	Unraveling Heat Transport and Dissipation in Suspended MoSe from Bulk to Monolayer.. <i>Advanced Materials</i> , 2022 , e2108352	24	1
57	Significant Increase of Electron Thermal Conductivity in Dirac Semimetal Beryllonitrene by Doping Beyond Van Hove Singularity. <i>Advanced Functional Materials</i> , 2111556	15.6	6
56	An Introduction to the Wonder 2D Nanomaterials: Synthetic Approaches and Fundamental Properties. <i>Materials Horizons</i> , 2022 , 1-24	0.6	
55	Ultralow thermal conductivity and anharmonic rattling in two-dimensional WB ₄ monolayer. <i>Applied Physics Letters</i> , 2022 , 120, 132202	3.4	1
54	Ternary pentagonal BNSi monolayer: Two-dimensional structure with potentially high carrier mobility and strong excitonic effects for photocatalytic applications. <i>Physical Review Materials</i> , 2022 , 6,	3.2	2
53	Enhanced thermoelectric properties of atomic-layer-deposited ZnO-Based superlattice thin films by tuning the composition and structure of interlayers. <i>Ceramics International</i> , 2022 , 48, 10202-10208	5.1	0
52	Measurement of Thermal Conductivity of Suspended and Supported Single-Layer WS ₂ Using Micro-photoluminescence Spectroscopy. <i>Journal of Physical Chemistry C</i> ,	3.8	1
51	High-performance thermoelectric properties of strained two-dimensional tellurium. <i>Physical Review Materials</i> , 2021 , 5,	3.2	0
50	Centimeter-Scale Synthesis of Monolayer WS ₂ Using Single-Zone Atmospheric-Pressure Chemical Vapor Deposition: A Detailed Study of Parametric Dependence, Growth Mechanism, and Photodetector Properties. <i>Crystal Growth and Design</i> ,	3.5	2
49	Theoretical investigations of Janus WSeTe monolayer and related van der Waals heterostructures with promising thermoelectric performance. <i>Applied Surface Science</i> , 2022 , 593, 153402	6.7	0
48	Ultrahigh Electron Thermal Conductivity in T-Graphene, Biphenylene, and Net-Graphene. <i>Advanced Energy Materials</i> , 2200657	21.8	4
47	Bilateral phonon transport modulation of Bi-layer TMDCs (MX ₂ , M=Mo, W; X=S). <i>International Journal of Thermal Sciences</i> , 2022 , 179, 107669	4.1	1
46	Biaxial strain tuned electronic structure, lattice thermal conductivity and thermoelectric properties of MgI ₂ monolayer. <i>Materials Science in Semiconductor Processing</i> , 2022 , 148, 106791	4.3	0
45	Thermal properties of single-layer MoS ₂ -WS ₂ alloys enabled by machine-learned interatomic potentials. <i>Chemical Communications</i> ,	5.8	0

44	Tunable lattice thermal conductivity of twisted bilayer MoS ₂ . <i>Physical Chemistry Chemical Physics</i> , 3.6	
43	First-Principles Study of the Optical Properties of TMDC/Graphene Heterostructures. <i>Photonics</i> , 2022 , 9, 387	2.2 0
42	Phase formation behavior and electronic transport properties of HfSe ₂ -HfTe ₂ solid solution system. <i>Journal of Alloys and Compounds</i> , 2022 , 166028	5.7 2
41	2D layered MSe ₂ (M = Hf, Ti and Zr) for compact lasers: nonlinear optical properties and GHz lasing. <i>Nanophotonics</i> , 2022 , 11, 3383-3394	6.3
40	Unravelling the thermoelectric properties and suppression of bipolar effect under strain engineering for the asymmetric Janus SnSSe and PbSSe monolayers. <i>Applied Surface Science</i> , 2022 , 599, 153962	6.7 2
39	Phase stability, phonon, electronic, and optical properties of not-yet-synthesized CsScS ₂ , CsYS ₂ , and APmS ₂ (A= Li, Na, K, Rb, Cs) materials: Insights from first-principles calculations. <i>Materials Science in Semiconductor Processing</i> , 2022 , 150, 106936	4.3 0
38	Reduction in thermal conductivity of monolayer WS ₂ caused by substrate effect.	0
37	Thermoelectric properties of the Janus PtSTe monolayer compared with its parent structures. 2022 , 6,	1
36	Thermal transport properties of monolayer GeS and SnS: A comparative study based on machine learning and SW interatomic potential models. 2022 , 12, 085111	1
35	Global structure search for new 2D PtSSe allotropes and their potential for thermoelectric and piezoelectric applications. 2022 , 805, 139913	1
34	BOLTZMANN TRANSPORT EQUATION FOR THERMAL TRANSPORT IN ELECTRONIC MATERIALS AND DEVICES. 2022 , 24, 131-172	0
33	Four-phonon and electron-phonon scattering effects on thermal properties in two-dimensional 2H-TaS ₂ . 2022 , 14, 13053-13058	0
32	Significantly suppressed thermal transport by doping In and Al atoms in gallium nitride. 2022 , 24, 21085-21093	0
31	First-principles study on phonon transport properties of MoTe ₂ and WTe ₂ monolayers in different phases. 2023 , 145, 115509	1
30	Phonon anharmonicity and thermal conductivity of two-dimensional van der Waals materials: A review. 2022 , 65,	0
29	Electronic and transport properties of semimetal ZrBeSi crystal: a first-principles study.	0
28	Terahertz resonance frequency through ethylene glycol phononic multichannel sensing via 2D MoS ₂ /PtSe ₂ structure. 2022 , 126863	1
27	Chromium ditelluride monolayer: A novel promising 2H phase thermoelectric material with direct bandgap and ultralow lattice thermal conductivity. 2022 , 167485	1

- 26 First-Principles Study of the Phonon Lifetime and Low Lattice Thermal Conductivity of Monolayer EGeSe: A Comparative Study. **2022**, 5, 15441-15448 ○
- 25 Anomalous Dynamics of Defect-Assisted Phonon Recycling in Few-Layer Mo_{0.5}W_{0.5}S₂. 10395-10403 ○
- 24 Stability of and conduction in single-walled Si₂BN nanotubes. **2022**, 6, ○
- 23 Interlayer Coupling Induced Phonon-Glass-Electron-Crystal Behavior in van der Waals Heterostructure PtSe₂/EGeSe. ○
- 22 High thermoelectric performance of a Sc₂Si₂Te₆ monolayer at medium temperatures: an ab initio study. ○
- 21 Strain engineering and thermoelectric performance of Janus monolayers of titanium dichalcogenides: A DFT study. **2023**, 218, 111925 ○
- 20 Thermoelectric performance and optoelectronic properties of Janus monolayer of ZrXY(X=E, D, S) (Y=E, S, Se). **2023**, 218, 111993 ○
- 19 Reconstruction of interfacial thermal transport mediated by hotspot in silicon-based nano-transistors. **2023**, 202, 123676 ○
- 18 Understanding the origins of low lattice thermal conductivity in a novel two-dimensional monolayer NaCuS for achieving medium-temperature thermoelectric applications. **2023**, 614, 156167 ○
- 17 Mechanism of the low thermal conductivity in novel two-dimensional NaCuSe. **2023**, 613, 156064 ○
- 16 Atomic Magnetic Heating Effect Enhanced Hydrogen Evolution Reaction of Gd@MoS₂ Single-Atom Catalysts. 2206155 ○
- 15 Two-dimensional Materials in the Display Industry: Status and Prospects. 2205520 ○
- 14 Chiral magnetism, lattice dynamics, and anomalous Hall conductivity in V₃AuN antiferromagnetic antiperovskite. **2022**, 6, ○
- 13 Accurate prediction on the lattice thermal conductivities of monolayer systems by a high-throughput descriptor. **2023**, 56, 045304 ○
- 12 Characterization of 2D transition metal dichalcogenides. **2023**, 97-139 ○
- 11 Janus EPdXY (X/Y = S, Se, Te) materials with high anisotropic thermoelectric performance. **2023**, 15, 5964-5975 ○
- 10 Thermal conductivity across transition metal dichalcogenide bilayers. **2023**, 26, 106447 ○
- 9 Phonon anharmonicity in Cu-based layered thiophosphates. **2023**, 35, 105840 ○

- 8 First-principles calculations to investigate structural and mechanical properties of MoS₂/MoSe₂ vertical and lateral Superlattice. **2023**, 45, 106234
- 7 Significantly reinforced thermoelectric performance in the novel 1T-Au₆Se₂ monolayer. **2023**, 11, 031103
- 6 Influence of embedded NiO-nanoparticles on the nonlinear absorption of tungsten disulfide nanolayers. **2023**, 138, 113657
- 5 Tensile strain and finite size modulation of low lattice thermal conductivity in monolayer TMDCs (HfSe₂ and ZrS₂) from first-principles: a comparative study. **2023**, 25, 9225-9237
- 4 Temporally probing the thermal phonon and charge transfer induced out-of-plane acoustical displacement of monolayer and bi-layer MoS₂/GaN heterojunction. **2023**, 30, 100477
- 3 First-principles investigation on the structural, vibrational, mechanical, electronic, and optical properties of MSi₂Z₄ (M : Pd and Pt, . **2023**, 7,
- 2 Emerging Versatile Two-Dimensional MoSi₂N₄ Family.
- 1 Structural, vibrational, electronic, and elastic properties of 2D alkali carbide as a metallic material. **2023**, e00805