

# CITATION REPORT

List of articles citing

Thermodynamic properties of PbTe, PbSe, and PbS:  
First-principles study

DOI: 10.1103/physrevb.80.024304  
Physical Review B, 2009, 80, .

**Source:** <https://exaly.com/paper-pdf/47055574/citation-report.pdf>

**Version:** 2024-04-26

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
217	Microstructure-Lattice Thermal Conductivity Correlation in Nanostructured PbTe <sub>0.7</sub> Sb <sub>0.3</sub> Thermoelectric Materials. <b>2010</b> , 20, 764-772		268
216	A study of electronic structure and lattice dynamics of CoSb <sub>3</sub> skutterudite. <b>2010</b> , 322, 3080-3083		21
215	Cooling effects of field emission from thermoelectric materials. <b>2010</b> ,		
214	On the origin of increased phonon scattering in nanostructured PbTe based thermoelectric materials. <i>Journal of the American Chemical Society</i> , <b>2010</b> , 132, 8669-75	16.4	177
213	P119: Cooling effects of field emission from PbTe. <b>2010</b> ,		
212	Thermoelectric transport properties of PbTe under pressure. <i>Physical Review B</i> , <b>2010</b> , 82,	3.3	82
211	High-temperature thermoelectric performance of heavily doped PbSe. <i>Physical Review B</i> , <b>2010</b> , 82,	3.3	216
210	Quasiparticle self-consistent GW calculations for PbS, PbSe, and PbTe: Band structure and pressure coefficients. <i>Physical Review B</i> , <b>2010</b> , 81,	3.3	122
209	STRUCTURAL, ELECTRONIC, OPTICAL AND THERMODYNAMIC PROPERTIES OF PbS, PbSe AND THEIR TERNARY ALLOY PbS <sub>1-x</sub> Sex. <b>2011</b> , 25, 473-486		8
208	Ultrafast demagnetization in ferromagnets and magnetic switching in nanoclusters when the number of photons is kept fixed. <b>2011</b> , 109, 07D303		8
207	Giant anharmonic phonon scattering in PbTe. <b>2011</b> , 10, 614-9		442
206	The Gruneisen parameter for silver azide. <b>2011</b> , 54, 765-772		2
205	Thermoelectric Properties of PbTe, SnTe, and GeTe at High Pressure: an Ab Initio Study. <b>2011</b> , 40, 641-647		43
204	Observation of regular defects formed on the surface of PbTe thin films grown by molecular beam epitaxy. <b>2011</b> , 257, 1986-1989		13
203	Anomalous lattice dynamics near the ferroelectric instability in PbTe. <b>2011</b> , 107, 175503		83
202	Thermal conductivity of half-Heusler compounds from first-principles calculations. <i>Physical Review B</i> , <b>2011</b> , 84,	3.3	163
201	Ab initio structure prediction for lead sulfide at standard and elevated pressures. <i>Physical Review B</i> , <b>2011</b> , 84,	3.3	56

200	Calculated electronic structure of $\text{Pb}_{1-x}\text{MnxTe}$ ( $0 \leq x$ ). <i>Physical Review B</i> , <b>2011</b> , 83,	3-3	29
199	Investigation of Structural Phase Transition of PbS. <b>2012</b> , 2012, 1-4		2
198	Microscopic mechanism of low thermal conductivity in lead telluride. <i>Physical Review B</i> , <b>2012</b> , 85,	3-3	101
197	Phase transition, elastic, and thermodynamic properties of NaF under high pressure. <b>2012</b> , 85, 409-418		1
196	Electron pairing and Coulomb repulsion in one-dimensional anharmonic lattices. <i>Physical Review B</i> , <b>2012</b> , 85,	3-3	23
195	Coherent and incoherent phase stabilities of thermoelectric rocksalt IV-VI semiconductor alloys. <i>Physical Review B</i> , <b>2012</b> , 86,	3-3	38
194	Elastic moduli and band gap of PbTe under pressure: ab initio study. <b>2012</b> , 28, 1308-1313		5
193	Molecular dynamics simulations of lattice thermal conductivity and spectral phonon mean free path of PbTe: Bulk and nanostructures. <b>2012</b> , 53, 278-285		133
192	Lattice dynamics of PbTe polymorphs from first principles. <b>2012</b> , 56, 18-24		9
191	Phonon conduction in PbSe, PbTe, and $\text{PbTe}_{1-x}\text{Sex}$ from first-principles calculations. <i>Physical Review B</i> , <b>2012</b> , 85,	3-3	368
190	Sterically active electron pairs in lead sulfide? An investigation of the electronic and vibrational properties of PbS in the transition region between the rock salt and the $\sqrt{2}\text{GeTe}$ -type modifications. <b>2012</b> , 18, 10929-36		29
189	Effects of surface structure and $\text{Ag}_{55}\text{Bi}$ nanodots on electronic properties of PbTe (100) facets from first-principles calculations. <b>2012</b> , 67, 17-20		2
188	Enthalpy of formation of Schottky defects in semiconductors. <b>2012</b> , 54, 1459-1462		6
187	Thermoelectric performance of PbSe quantum dot films. <i>Nanoscale</i> , <b>2013</b> , 5, 7290-6	7-7	25
186	First Principles Study of Structural, Magnetic and Electronic Properties of $\text{PbX}$ ( $\text{X} = \text{S}$ and $\text{Se}$ ) Doped with B, C and N. <b>2013</b> , 26, 3437-3442		4
185	Lattice contribution to the high dielectric constant of PbTe. <i>Physical Review B</i> , <b>2013</b> , 87,	3-3	17
184	Sound velocities of PbTe to 14 GPa: evidence for coupling between acoustic and optic phonons. <b>2013</b> , 25, 365402		5
183	Direct Evidence of Cation Disorder in Thermoelectric Lead Chalcogenides PbTe and PbS. <b>2013</b> , 23, 5477-5483		83

182	Photoinduced features of energy bandgap in quaternary Cu <sub>2</sub> CdGeS <sub>4</sub> crystals. <b>2013</b> , 25, 505802	14
181	Structural aspects of changes induced in PbTe by doping with Mn, In and Ga. <b>2013</b> , 48, 8084-8100	8
180	Phase transitions in PbTe under quasi-hydrostatic pressure up to 50 GPa. <b>2013</b> , 33, 713-719	10
179	First-principles investigation of dual substitutional impurity-induced electronic structural modulation of PbTe on cationic and anionic sites. <b>2013</b> , 61, 6428-6442	2
178	STRUCTURAL, ELECTRONIC, MAGNETIC AND OPTICAL PROPERTIES OF FERROMAGNETIC Pb <sub>1-x</sub> Eu <sub>x</sub> Se AND Pb <sub>1-x</sub> Eu <sub>x</sub> Te ALLOYS (x = 0, 0.25, 0.50, 0.75 AND 1). <b>2013</b> , 27, 1350100	5
177	Simulating realistic imaging conditions for in situ liquid microscopy. <b>2013</b> , 135, 36-42	15
176	New exploration on phase transition and structure of PbS under high pressure and temperature. <b>2013</b> , 113, 043509	2
175	Pressure-Induced Superconductivity in SnTe: A First-Principles Study. <b>2013</b> , 117, 12266-12271	24
174	DFT+U study of the structural and electronic properties of the ferromagnetic and antiferromagnetic ordering in the PbS-based ternary alloys Pb <sub>1-x</sub> Eu <sub>x</sub> S (x = 0.25, 0.50, 0.75 and 1). <b>2013</b> , 18, 24-35	8
173	Phase-transition induced elastic softening and band gap transition in semiconducting PbS at high pressure. <b>2013</b> , 52, 8638-43	24
172	Pressure-Driven Enhancement of Topological Insulating State in Tin Telluride. <b>2013</b> , 117, 8437-8442	15
171	Cross-plane thermal conductivity temperature dependence for PbSnSe/PbSe thin film superlattice material from 100K to 300K. <b>2013</b> , 1456, 51	
170	Alkaline earth lead and tin compounds AePb, AeSn, Ae = Ca, Sr, Ba, as thermoelectric materials. <b>2013</b> , 14, 055003	14
169	Electronic Structure, Lattice Dynamics and Thermoelectric Properties of PbTe from First-Principles Calculation. <b>2013</b> , 30, 017101	6
168	Origin of anomalous anharmonic lattice dynamics of lead telluride. <b>2014</b> , 7, 041801	19
167	Temperature effects on the energy bandgap and conductivity effective masses of charge carriers in lead telluride from first-principles calculations. <b>2014</b> , 116, 013708	4
166	Structure determination of the intermediate phase of PbSe using experiments and calculations. <b>2014</b> , 116, 053502	2
165	Significant lattice thermal conductivity reduction following phase separation of the highly efficient GexPb <sub>1-x</sub> Te thermoelectric alloys. <b>2014</b> , 251, 1431-1437	70

164	Anharmonic effects in the thermoelectric properties of PbTe. <b>2014</b> , 116, 043702		9
163	Thermal expansion of nanostructured PbS films and anharmonicity of atomic vibrations. <b>2014</b> , 56, 2353-2358		13
162	Structures of two intermediate phases between the B1 and B2 phases of PbS under high pressure. <b>2014</b> , 4, 127112		7
161	Contrasting role of antimony and bismuth dopants on the thermoelectric performance of lead selenide. <b>2014</b> , 5, 3640		76
160	Effect of particle size on the thermal expansion of nanostructured lead sulfide films. <i>Journal of Alloys and Compounds</i> , <b>2014</b> , 610, 196-202	5-7	23
159	Study of lattice thermal conductivity of PbS. <i>Journal of Alloys and Compounds</i> , <b>2014</b> , 584, 381-384	5-7	5
158	First-principle calculation and quasi-harmonic Debye model prediction for elastic and thermodynamic properties of Bi <sub>2</sub> Te <sub>3</sub> . <b>2014</b> , 82, 45-49		24
157	First principles calculations of structural, electronic and thermal properties of lead chalcogenides PbS, PbSe and PbTe compounds. <b>2014</b> , 37, 1159-1166		9
156	First-principles approach to nonlinear lattice dynamics: anomalous spectra in PbTe. <b>2014</b> , 113, 105501		37
155	Resonant bonding leads to low lattice thermal conductivity. <b>2014</b> , 5, 3525		374
154	Chemical composition tuning in quaternary p-type Pb-chalcogenides--a promising strategy for enhanced thermoelectric performance. <b>2014</b> , 16, 1835-40		46
153	Polar effects on the thermal conductivity of cubic boron nitride under pressure. <b>2014</b> , 113, 025901		26
152	Temperature and pressure behaviour of narrow-gap semiconductors including galena. <b>2014</b> , 14, 496-507		4
151	Thermal physics of the lead chalcogenides PbS, PbSe, and PbTe from first principles. <i>Physical Review B</i> , <b>2014</b> , 89,	3-3	172
150	Ab-Initio Determination of Pressure-Dependent Electronic and Optical Properties of Lead Sulfide for Energy Applications. <b>2014</b> , 327-344		1
149	Vibrational contributions to the phase stability of PbS-PbTe alloys. <i>Physical Review B</i> , <b>2015</b> , 92,	3-3	15
148	Influence of the exchange-correlation functional on the quasi-harmonic lattice dynamics of II-VI semiconductors. <b>2015</b> , 143, 064710		60
147	Origin of resistivity anomaly in p-type leads chalcogenide multiphase compounds. <b>2015</b> , 5, 053601		8

146	The role of acoustic phonon anharmonicity in determining thermal conductivity of CdSiP <sub>2</sub> and AgGaS <sub>2</sub> : First principles calculations. <b>2015</b> , 5, 127236		8
145	Thermoelectric properties of rocksalt ZnO from first-principles calculations. <b>2015</b> , 118, 165101		11
144	Heterogeneous Distribution of Sodium for High Thermoelectric Performance of p-type Multiphase Lead-Chalcogenides. <b>2015</b> , 5, 1501047		56
143	Raman scattering in lead selenide films at a low excitation level. <b>2015</b> , 119, 938-942		5
142	Determining dilute-limit solvus boundaries in multi-component systems using defect energetics: Na in PbTe and PbS. <i>Journal of Materials Chemistry C</i> , <b>2015</b> , 3, 10630-10649	7.1	18
141	First-principles study on the lattice dynamics and thermodynamic properties of Cu <sub>2</sub> GeSe <sub>3</sub> . <b>2015</b> , 109, 47004		16
140	High-Pressure Phase Transitions of PbTe Using the First-Principles Calculations. <b>2015</b> , 32, 016101		3
139	Theoretical understanding on band engineering of Mn-doped lead chalcogenides PbX (X = Te, Se, S). <b>2015</b> , 27, 095501		19
138	Taking steps forward in understanding the electrochemical behavior of Na <sub>2</sub> Ti <sub>3</sub> O <sub>7</sub> . <i>Journal of Materials Chemistry A</i> , <b>2015</b> , 3, 22280-22286	13	37
137	Structural, Electronic, Elastic and Thermal Properties of Li <sub>2</sub> AgSb: First-Principles Calculations. <b>2015</b> , 70, 611-618		
136	Reconstructions and stabilities of PbTe(1 1 1) crystal surface from experiments and density-functional theory. <b>2015</b> , 356, 742-746		5
135	Lattice-mismatched heteroepitaxy of IV-VI thin films on PbTe(001): An ab initio study. <i>Physical Review B</i> , <b>2015</b> , 91,	3.3	6
134	Towards a predictive route for selection of doping elements for the thermoelectric compound PbTe from first-principles. <b>2015</b> , 117, 175102		14
133	Thermoelectric properties of single-layered SnSe sheet. <i>Nanoscale</i> , <b>2015</b> , 7, 15962-70	7.7	181
132	The role of point defects in PbS, PbSe and PbTe: a first principles study. <b>2015</b> , 27, 355801		15
131	Phonon transport in perovskite SrTiO <sub>3</sub> from first principles. <b>2015</b> , 8, 071501		44
130	Model calculation and experimental identification of nanocrystalline Li <sub>2</sub> C <sub>2</sub> as cathode material for lithium-ion battery. <b>2015</b> , 186, 512-521		9
129	Ab initio investigations of electron correlation effect and phonon dynamics of orthorhombic uranium. <b>2015</b> , 252, 521-531		6

128	Enhancing Thermoelectric Performance of PbTe-Based Compounds by Substituting Elements: A First Principles Study. <b>2015</b> , 44, 1460-1468		18
127	One-step bonding of Ni electrode to n-type PbTe [A step towards fabrication of thermoelectric generators. <b>2016</b> , 107, 90-97		26
126	On the tuning of electrical and thermal transport in thermoelectrics: an integrated theoryExperiment perspective. <b>2016</b> , 2,		290
125	Elastic constant C11 of 12C diamond between 10 and 613 K. <b>2016</b> , 108, 221902		5
124	Optic phonons and anisotropic thermal conductivity in hexagonal GeSbTe. <b>2016</b> , 6, 37076		30
123	Ultrafast lattice dynamics in lead selenide quantum dot induced by laser excitation. <b>2016</b> , 109, 153105		9
122	Harmonic phonon theory for calculating thermal conductivity spectrum from first-principles dispersion relations. <b>2016</b> , 108, 201903		7
121	Stabilities and Reconstructions of Clean PbS and PbSe Surfaces: DFT Results and the Role of Dispersion Forces. <b>2016</b> , 120, 8813-8820		13
120	Enhanced thermoelectric performance in PbSe-SrSe solid solution by Mn substitution. <i>Journal of Alloys and Compounds</i> , <b>2016</b> , 687, 765-772	5:7	13
119	A first-principles study on the intrinsic phonon transport of Cu <sub>2</sub> GeSe <sub>3</sub> . <b>2016</b> , 115, 26002		4
118	First-principles DebyeCallaway approach to lattice thermal conductivity. <b>2016</b> , 2, 237-247		34
117	Lattice thermal conductivity in layered BiCuSeO. <b>2016</b> , 18, 19158-64		23
116	Electronic Structure and Transport Properties of Doped Lead Chalcogenides from First Principles. <b>2016</b> , 1, 4003-4010		1
115	Anharmonicity in the High-Temperature Cmc <sub>2</sub> m Phase of SnSe: Soft Modes and Three-Phonon Interactions. <b>2016</b> , 117, 075502		104
114	A Joint Computational and Experimental Evaluation of CaMn <sub>2</sub> O <sub>4</sub> Polymorphs as Cathode Materials for Ca Ion Batteries. <i>Chemistry of Materials</i> , <b>2016</b> , 28, 6886-6893	9.6	64
113	Phonons. <b>2016</b> , 230-250		
112	Theoretical Model of Thermoelectric Transport Properties. <b>2016</b> , 286-322		
111	Broadband phonon scattering in PbTe-based materials driven near ferroelectric phase transition by strain or alloying. <i>Physical Review B</i> , <b>2016</b> , 93,	3:3	22

110	Benchmarking density functional perturbation theory to enable high-throughput screening of materials for dielectric constant and refractive index. <i>Physical Review B</i> , <b>2016</b> , 93,	3-3	33
109	A first-principles study on the phonon transport in layered BiCuOSe. <b>2016</b> , 6, 21035		44
108	Non-equilibrium processing leads to record high thermoelectric figure of merit in PbTe-SrTe. <b>2016</b> , 7, 12167		377
107	First-principles study on the thermal expansion of Ni-X binary alloys based on the quasi-harmonic Debye model. <b>2016</b> , 22, 1065-1072		6
106	Ab initio calculation of pentacene-PbSe hybrid interface for photovoltaic applications. <b>2016</b> , 18, 18209-18		4
105	A Theoretical Model of Thermoelectric Transport Properties for Electrons and Phonons. <b>2016</b> , 45, 1115-1141		10
104	Thermoelectric studies of IV-VI semiconductors for renewable energy resources. <b>2016</b> , 48, 85-94		36
103	Predicting Single-Layer Technetium Dichalcogenides (TcX <sub>2</sub> = S, Se) with Promising Applications in Photovoltaics and Photocatalysis. <b>2016</b> , 8, 5385-92		78
102	Calculation of dopant solubilities and phase diagrams of X <sub>2</sub> Pb <sub>2</sub> Se (X = Br, Na) limited to defects with localized charge. <i>Journal of Materials Chemistry C</i> , <b>2016</b> , 4, 1769-1775	7-1	8
101	Structural stability and thermoelectric property optimization of Ca <sub>2</sub> Si. <b>2017</b> , 7, 8936-8943		9
100	Phonon transport in Na <sub>2</sub> He at high pressure from a first-principles study. <b>2017</b> , 110, 172104		5
99	Effect of lattice relaxation on thermal conductivity of fcc-based structures: an efficient procedure of molecular dynamics simulation. <b>2017</b> , 25, 055011		3
98	n-type Bi-doped PbTe Nanocubes with Enhanced Thermoelectric Performance. <b>2017</b> , 31, 105-112		84
97	Improving Thermoelectric Performance of BiMgAgSb by Theoretical Band Engineering Design. <b>2017</b> , 7, 1700076		32
96	Broadband Cooling Spectra of Hot Electrons and Holes in PbSe Quantum Dots. <b>2017</b> , 11, 6286-6294		31
95	Intrinsic localized mode and low thermal conductivity of PbSe. <i>Physical Review B</i> , <b>2017</b> , 95,	3-3	54
94	First-principles calculation of intrinsic defect chemistry and self-doping in PbTe. <b>2017</b> , 3,		43
93	Evolution of phonon anharmonicity in Se-doped Sb <sub>2</sub> Te <sub>3</sub> thermoelectrics. <i>Physical Review B</i> , <b>2017</b> , 96,	3-3	12



92	Investigations of press-induced band gap changes in PbS. <b>2017</b> , 687, 101-105		4
91	Remarkable Roles of Cu To Synergistically Optimize Phonon and Carrier Transport in n-Type PbTe-CuTe. <i>Journal of the American Chemical Society</i> , <b>2017</b> , 139, 18732-18738	16.4	179
90	Lattice thermal transport in La <sub>3</sub> Cu <sub>3</sub> X <sub>4</sub> compounds (X=P,As,Sb,Bi): Interplay of anharmonicity and scattering phase space. <i>Physical Review B</i> , <b>2017</b> , 95,	3.3	11
89	Main-Group Halide Semiconductors Derived from Perovskite: Distinguishing Chemical, Structural, and Electronic Aspects. <b>2017</b> , 56, 11-25		36
88	A Practical Approach to Evaluate Lattice Thermal Conductivity in Two-Phase Thermoelectric Alloys for Energy Applications. <b>2017</b> , 10,		8
87	Structural stability, dynamical stability, thermoelectric properties, and elastic properties of GeTe at high pressure. <i>Physical Review B</i> , <b>2018</b> , 97,	3.3	29
86	Thermoelectric Performance of Single Phase p-Type Quaternary (PbTe) <sub>0.65</sub> (PbSe) <sub>0.35</sub> (PbS) <sub>x</sub> Alloys. <b>2018</b> , 1, 1898-1903		5
85	Computational prediction of a high ZT of n-type MgSb-based compounds with isotropic thermoelectric conduction performance. <b>2018</b> , 20, 7686-7693		38
84	Thermoelectric transport properties of rock-salt SnSe: first-principles investigation. <i>Journal of Materials Chemistry C</i> , <b>2018</b> , 6, 12016-12022	7.1	22
83	Synthesis of In <sub>2</sub> S <sub>3</sub> thin films directly onto conductive substrates via PVP-assisted microwave irradiation method. <b>2018</b> , 210, 66-69		10
82	Free energy, configurational and nonextensivity of Tsallis entropy with the size and temperature in colloidal silver nanoparticles in [EMim][PF <sub>6</sub> ] ionic liquid. <b>2018</b> , 249, 1012-1019		1
81	Tuning electronic and magnetic properties of V-, Cr-, and Mn-doped PbS via strain engineering: A first-principles proposal. <b>2018</b> , 228, 1-6		8
80	Designing high-performance n-type Mg <sub>3</sub> Sb <sub>2</sub> -based thermoelectric materials through forming solid solutions and biaxial strain. <i>Journal of Materials Chemistry A</i> , <b>2018</b> , 6, 20454-20462	13	19
79	Modulation of thermal conductivity and thermoelectric figure of merit by anharmonic lattice vibration in Sb <sub>2</sub> Te <sub>3</sub> thermoelectrics. <b>2018</b> , 8, 125119		2
78	Ab initio phase diagram of PbSe crystals calculated with the random phase approximation. <i>Physical Review B</i> , <b>2018</b> , 98,	3.3	2
77	Constructing Highly Porous Thermoelectric Monoliths with High-Performance and Improved Portability from Solution-Synthesized Shape-Controlled Nanocrystals. <b>2018</b> , 18, 4034-4039		25
76	Revisiting PbTe to identify how thermal conductivity is really limited. <i>Physical Review B</i> , <b>2018</b> , 97,	3.3	21
75	Thermoelectric properties of p-type cubic and rhombohedral GeTe. <b>2018</b> , 123, 195105		33

74	Lattice anharmonicity, phonon dispersion, and thermal conductivity of PbTe studied by the phonon quasiparticle approach. <i>Physical Review B</i> , <b>2018</b> , 97,	3-3	21
73	Thermoelectric Performance of IV-VI Compounds with Octahedral-Like Coordination: A Chemical-Bonding Perspective. <b>2018</b> , 30, e1801787		54
72	Fabrication, characterization and simulation of Zn-doped PbS nanopowder. <b>2018</b> , 545, 245-249		5
71	Low Temperature Synthesis as a Route for Highly Thermoelectric Efficient Na-Doped PbTe. <b>2018</b> , 215, 1800098		1
70	Phonon band gaps in the IV-VI monochalcogenides. <i>Physical Review B</i> , <b>2019</b> , 100,	3-3	11
69	The Thermal Expansion of Ag <sub>x</sub> Pb <sub>1-x</sub> S Limited Semiconductor Solid Solutions. <b>2019</b> , 61, 982-986		
68	Growth of quantum dot coated core-shell anisotropic nanowires for improved thermal and electronic transport. <b>2019</b> , 114, 243104		5
67	Recent progress in fundamental understanding of halide perovskite semiconductors. <b>2019</b> , 106, 100580		69
66	Single-layer CdPSe <sub>3</sub> : A promising thermoelectric material persisting in high temperatures. <b>2019</b> , 115, 193105		3
65	Thermal Expansion of Nanostructured Solid Solutions of Lead and Silver Sulfides. <b>2019</b> , 18, 1940061		1
64	Thermally enhanced Fröhlich coupling in SnSe. <i>Physical Review B</i> , <b>2019</b> , 99,	3-3	10
63	Theoretical Investigation of Metal-Shrouded Tl <sub>2</sub> O Monolayers: Pudding-Mold-Type Band Structure and Thermoelectric Performance. <b>2019</b> , 2, 4061-4066		15
62	Bandlike Transport in PbS Quantum Dot Superlattices with Quantum Confinement. <b>2019</b> , 10, 3756-3762		6
61	Ultralow Lattice Thermal Conductivity and Thermoelectric Properties of Monolayer Tl <sub>2</sub> O. <b>2019</b> , 2, 3004-3008		29
60	Carrier tuning and multiple phonon scattering induced high thermoelectric performance in n-type Sb-doped PbTe alloys. <b>2019</b> , 125, 1		9
59	High-performance electron-doped GeMnTe <sub>2</sub> : hierarchical structure and low thermal conductivity. <i>Journal of Materials Chemistry A</i> , <b>2019</b> , 7, 27361-27366	13	10
58	Effects of Doping of Lead Sulfide with Silver on the Lattice and Optical Properties of Pb <sub>1-x</sub> Ag <sub>x</sub> S Solid Solutions. <b>2019</b> , 53, 1665-1671		1
57	Influences of isotropic strain on the electronic and magnetic properties of Fe-, Co-, and Ni-doped PbS revealed by density functional calculations. <b>2019</b> , 223, 133-139		1

56	Physical Properties of Sn-Doped PbSe Nanostructures as Photovoltaic Application. <b>2020</b> , 30, 986-993		2
55	Chalcogenide Thermoelectrics Empowered by an Unconventional Bonding Mechanism. <b>2020</b> , 30, 1904862		88
54	Structural, Electronic and Thermoelectric Properties of $Pb_{1-x}Sn_xTe$ Alloys. <b>2020</b> , 49, 586-592		3
53	Structure, elastic characteristic, ideal strengths, and phonon stability of binary uranium intermetallic UGe of AuCu-type. <b>2020</b> , 22, 1381-1391		1
52	High Thermoelectric Performance of New Two-Dimensional IV <sup>VI</sup> Compounds: A First-Principles Study. <b>2020</b> , 124, 1812-1819		25
51	Thermal Conductivity of HfTe5: A Critical Revisit. <b>2020</b> , 30, 1907286		6
50	Monolayer Ag2S: Ultralow Lattice Thermal Conductivity and Excellent Thermoelectric Performance. <b>2020</b> , 3, 10147-10153		3
49	Effect of impurities and defect in thermal conductivity of lead sulphide. <b>2020</b> , 94, 1		
48	Intrinsically Ultralow Thermal Conductivity in Ruddlesden-Popper 2D Perovskite CsPbCl <sub>3</sub> : Localized Anharmonic Vibrations and Dynamic Octahedral Distortions. <i>Journal of the American Chemical Society</i> , <b>2020</b> , 142, 15595-15603	16.4	44
47	Optimized Strategies for Advancing n-Type PbTe Thermoelectrics: A Review. <b>2020</b> , 12, 49323-49334		17
46	High-throughput computational screening of 2D materials for thermoelectrics. <i>Journal of Materials Chemistry A</i> , <b>2020</b> , 8, 19674-19683	13	10
45	Phonon-Driven Energy Relaxation in PbS/CdS and PbSe/CdSe Core/Shell Quantum Dots. <b>2020</b> , 11, 4269-4278		7
44	Thermoelectric properties of monolayer GeAsSe and SnSbTe. <i>Journal of Materials Chemistry C</i> , <b>2020</b> , 8, 9763-9774	7.1	12
43	Investigation of the Thermal Properties and Crystal Growth of the Nonlinear Optical Crystals AgGaS <sub>2</sub> and AgGaGeS <sub>4</sub> . <b>2020</b> , 20, 3140-3153		6
42	Graphene/ZnO van der Waals Stacks for Thermal Management. <b>2020</b> , 3, 7136-7142		0
41	Lattice dynamics of Pnma Sn(S <sub>1-x</sub> Se <sub>x</sub> ) solid solutions: energetics, phonon spectra and thermal transport. <b>2020</b> , 2, 025006		3
40	Band Sharpening and Band Alignment Enable High Quality Factor to Enhance Thermoelectric Performance in n-Type PbS. <i>Journal of the American Chemical Society</i> , <b>2020</b> , 142, 4051-4060	16.4	71
39	Effect of intrinsic defects on the thermal conductivity of PbTe from classical molecular dynamics simulations. <b>2020</b> , 32, 045701		6

38	Optimization and modulation for the moderate and high temperature thermoelectric properties of PbSe via solid solution with PbS synthesized by HPHT. <b>2020</b> , 34, 2050185	3
37	Band flattening and phonon-defect scattering in cubic SnSeAgSbTe <sub>2</sub> alloy for thermoelectric enhancement. <b>2021</b> , 16, 100298	8
36	The mechanical and thermal properties of (Th,U)Si compounds: A systematic density functional theory research. <b>2021</b> , 188, 110148	4
35	Multicarrier Dynamics in Quantum Dots. <b>2021</b> , 121, 2325-2372	28
34	Origins of low lattice thermal conductivity of PbSnTe alloys for thermoelectric applications. <b>2021</b> , 50, 4323-4334	10
33	Hydrostatic Pressure Tuning of Thermal Conductivity for PbTe and PbSe Considering Pressure-Induced Phase Transitions. <b>2021</b> , 6, 3980-3990	4
32	Finite-temperature materials modeling from the quantum nuclei to the hot electron regime. <b>2021</b> , 5,	4
31	The Verification of Thermoelectric Performance Obtained by High-Throughput Calculations: The Case of GeS <sub>2</sub> Monolayer From First-Principles Calculations. <b>2021</b> , 8,	2
30	Novel thermoelectric performance of 2D 1T- SeTe and SeTe with ultralow lattice thermal conductivity but high carrier mobility. <b>2021</b> , 32,	4
29	Thermostructural and Elastic Properties of PbTe and Pb <sub>0.884</sub> Cd <sub>0.116</sub> Te: A Combined Low-Temperature and High-Pressure X-ray Diffraction Study of Cd-Substitution Effects. <b>2021</b> , 11, 1063	0
28	Nanostructured Lead Sulfide PbS. <b>2018</b> , 31-126	1
27	Synergistic tuning of carrier mobility, effective mass, and point defects scattering triggered high thermoelectric performance in n-type Ge-doped PbTe. <b>2019</b> , 125, 055104	3
26	Controlling phonon lifetimes via sublattice disordering in AgBiSe <sub>2</sub> . <b>2020</b> , 4,	3
25	Semiempirical Energies of Vacancy Formation in Semiconductors. <b>2016</b> , 61, 992-1007	4
24	Ab initio calculation of phase transitions, elastic, and thermodynamic properties of MnPd alloys. <b>2012</b> , 61, 246201	1
23	Mixed-Valence CsCuSe: Large Phonon Anharmonicity Driven by the Hierarchy of the Rigid [(Cu)(Se)](Se) Double Anti-CaF Layer and the Soft Cs Sublattice. <i>Journal of the American Chemical Society</i> , <b>2021</b> , 143, 18490-18501	16.4 3
22	Pressure and doping effects on the structural stability of thermoelectric BaAgTe. <b>2021</b> , 34,	
21	First-Principle Investigations on the Electronic and Transport Properties of PbBiTeX (X = S/Se/Te) Monolayers. <b>2021</b> , 11,	

20	Ultrahigh Power Factor and Ultralow Thermal Conductivity at Room Temperature in PbSe/SnSe Superlattice: Role of Quantum-Well Effect. <b>2021</b> , e2104916		2
19	The coexistence of superior intrinsic piezoelectricity and thermoelectricity in two-dimensional Janus $\text{TeSSe}$ . <b>2021</b> , 23, 26955-26966		1
18	Low-intermediate-temperature, high-pressure thermoelastic and crystallographic properties of thermoelectric clausthalite (PbSe-I).		
17	Low thermal conductivity in franckeite heterostructures.. <i>Nanoscale</i> , <b>2022</b> ,	7.7	
16	Slow Excitonic Carrier Cooling in Sr-doped PbS Nanocrystals for Hot Carrier Devices: Integrated Experimental and First-principles Approach. <i>Journal of Materials Chemistry C</i> ,	7.1	0
15	Giant Modulation of the Electron Mobility in Semiconductor BiOSe via Incipient Ferroelectric Phase Transition.. <i>Journal of the American Chemical Society</i> , <b>2022</b> ,	16.4	3
14	Intrinsically Low Thermal Conductivity in the n-Type Vacancy-Ordered Double Perovskite Cs <sub>2</sub> SnI <sub>6</sub> : Octahedral Rotation and Anharmonic Rattling. <i>Chemistry of Materials</i> ,	9.6	7
13	Honeycomb-like puckered PbTe monolayer: A promising n-type thermoelectric material with ultralow lattice thermal conductivity. <i>Journal of Alloys and Compounds</i> , <b>2022</b> , 907, 164439	5.7	1
12	PbTe/PbSe Thermoelectric Nanocomposites: The Impact of Length Modulations on Lowering Thermal Conductivity. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> ,	1.3	0
11	Thermoelectric Materials. <b>2022</b> , 509-665		
10	Y <sub>2</sub> Ti <sub>2</sub> O <sub>5</sub> S <sub>2</sub> is a promising n-type oxysulphide for thermoelectric applications. <i>Journal of Materials Chemistry A</i> ,	13	1
9	Glassy thermal conductivity in Cs <sub>3</sub> Bi <sub>2</sub> I <sub>6</sub> Cl <sub>3</sub> single crystal. <b>2022</b> , 13,		4
8	Physical characteristics of Pb <sub>1-x</sub> A <sub>x</sub> Se (A=Fe, Mn, V) for spintronic applications. <b>2022</b> , 19, 553-563		0
7	Carbon-based monochalcogenides for efficient solar and heat energy harvesting. <b>2023</b> , 608, 155121		0
6	Ab Initio Study of Carrier Mobility, Thermodynamic and Thermoelectric Properties of Kesterite Cu <sub>2</sub> ZnGeS <sub>4</sub> . <b>2022</b> , 23, 12785		1
5	Interlayer Coupling Induced Phonon-Glass/Electron-Crystal Behavior in van der Waals Heterostructure PtSe <sub>2</sub> /EGeSe.		0
4	First-principles calculations of the dynamical and thermodynamic properties of lead chalcogenides PbX (X = S, Se, Te). <b>2022</b> , 19, 793-803		0
3	Correlation between spontaneous polarization and thermal conductivity in ferroelectric HfO <sub>2</sub> from first principles. <b>2023</b> , 207, 123971		0

- 2 Phonon transport in  $\text{Cu}_2\text{GeSe}_3$  : Effects of spin-orbit coupling and higher-order phonon-phonon scattering. **2023**, 107, ○
- 1 Doping by Design: Enhanced Thermoelectric Performance of GeSe Alloys Through Metavalent Bonding. ○