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## **BOB - CABRERA BRUNO**

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### **Phonon properties and thermal conductivity from first ...**

The linear phonon dispersion of Debye offers many simplifications on phonon transport properties, and was the most common approximation in the past century. The linear dispersion of Debye... We report results of investigation of the phonon and thermal properties of the exfoliated films of layered single crystals of antiferromagnetic FePS<sub>3</sub> and MnPS<sub>3</sub> semiconductors. Raman spectroscopy was conducted using three different excitation lasers with wavelengths of 325 nm (UV), 488 nm (blue), and 633 nm (red). UV-Raman spectroscopy reveals spectral features which are not detectable via ...

The phonon band structures and the partial density of states are

also investigated, and we find that both CsBi<sub>4</sub>Te<sub>6</sub> and Bi<sub>2</sub>Te<sub>3</sub> exhibit localized phonon states at low frequencies. At high temperatures, the decrease of the volume expansion with temperature indicates the potential of a good thermal conductivity in this temperature region.

### **Ab initio calculations of the thermal properties of boron ...**

The thermal conductivity is then expressed as: where is the volume of the unit cell, N the number of -points used in the sampling, the Bose-Einstein distribution function,, and correspond to the phonon frequency, velocity and relaxation time respectively. The term captures the deviation on the heat current with respect to the RTA approach.

### **Enhanced thermal conduction by surface phonon-polaritons ...**

Thermal conductivity Phonons and thermal conductivity Phonons

have energy and momentum and, therefore, can conduct heat. Kinetic theory gives the thermal conductivity Excess temperature of phonons crossing plane Excess energy of each phonon  $\hbar \omega$   $dz$   $dT$   $dz$   $dT$   $DT = D = \hbar \omega dz$   $dT$   $c$   $phDT = -c$   $ph$   $l$   $q$   $z$   $Dz = -l$   $\cos$   $q$  heat capacity of a phonon heat capacity of a phonon

We investigated the vibrational property of lead telluride (PbTe) with a focus on lattice anharmonicity at moderate temperatures (300 < T < 800 K) using the phonon quasiparticle approach which combines first-principles molecular dynamics and lattice dynamics. The calculated anharmonic phonon dispersions are strongly temperature dependent and some phonon modes adopt giant frequency shifts, e.g ...

Thermal properties in the harmonic approximation¶. This section of the tutorial demonstrates how an existing FCP can be employed in conjunction with phonopy to analyze the thermal properties of a material in the harmonic approximation.. Note that this analysis by definition invokes only the second-order force constants and primarily relies on phonopy.

[nanoHUB-U Thermal Energy at the Nanoscale L3.2: Basic Thermal Properties - Acoustic Phonon Sp. Heat](#) **Skoltech Colloquium: Phonon Transport in Graphene with Prof Balandin, 30.06.2014** [Thermal Conductivity {Texas A\u0026M: Intro to Materials} Thermal properties](#) [nanoHUB-U Thermal Energy at the Nanoscale L3.3: Basic Thermal Properties - Optical Phonon Sp. Heat](#) [Phonon Calculations in Materials Science using VASP \u0026 phonopy](#) [Near-equilibrium Transport Lecture 9: Phonon Transport](#)

~~Nanomanufacturing: 06— Thermal properties of nanostructures Thermal properties of materials Mod-01 Lec-14 Lattice Vibrations (Continued) Phonon thermal conductivity THERMAL PROPERTIES Thermal conductivity and phonon collisions 172 - Phonons. Phonons at Surfaces (VintageVideo) Making sense of Brillouin Zones - Part 1 Dynamic Control of Phonon Propagation in Phononic Crystal Waveguide PHYS 201 | Dispersion 3 - Reading Dispersion Curves Solid State Physics in a Nutshell: Week 5.1 Introduction to Phonons How to measure heat flux? Thermal Expansion {Texas A\u0026M: Intro to Materials} Electron - Phonon Interaction (Simple) Thermal Expansion {Texas A\u0026M: Intro to Materials (MSEN 201)} Introduction to Solid State Physics, Lecture 5: One-dimensional models of vibrations in solids Phonon thermal transport in 2D materials - LUCAS LINDSAY Solid State Physics in a Nutshell: Topic 6-3: Thermal Conductivity Understanding what is Thermal Conductivity? PHONONS N-PROCESS U-PROCESS (HINDI) lec-25 nanoHUB-U Thermal Energy at the Nanoscale L5.3: Carrier Scattering - Phonon-Phonon Scattering MSN 514 - Lecture 32: Phonons and stability nanoHUB-U Thermoelectricity L2.5: Thermoelectric Transport Parameters - Lattice Thermal Conductivity Thermal Properties And Phonon Dispersion Thermal Properties and Phonon Spectral Characterization of ... Thermal Properties and Phonon Spectral Characterization of Synthetic Boron Phosphide for High Thermal Conductivity Applications. ... Materials Discovery and Properties Prediction in Thermal Transport via Materials Informatics: A Mini Review. Nano Letters 2019, 19 (6) , 3387-3395. DOI: 10.1021/acs.nanolett.8b05196. ...~~

It is noted here that the lattice thermal conductivity and phonon dispersion relation are sensitive to strain, which further confirms that different treatments on optimized lattice constants lead to a significant difference on the lattice thermal conductivity and phonon dispersion relation.

### **Theory of Phonon Thermal Transport in Graphene and Graphite**

#### **Rationalizing phonon dispersion: an efficient and precise**

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The most fundamental thermal properties of solids can be determined from the phonon dispersion  $q, \nu(q)$  (for wave vector  $q$  of the  $\nu$ th mode) and the corresponding phonon density of states (DOS) as a function of frequency. The Helmholtz free energy at the temperature  $T$  and for a constant volume  $V$  is given by  $F(T, V) = -k_B T \ln Z$

Improving heat dissipation in increasingly miniature microelectronic devices is a serious challenge, as the thermal conduction in nanostructures is markedly reduced by increasingly frequent scattering of phonons on the surface. However, the surface could become an additional heat dissipation channel if phonons couple with photons forming hybrid surface quasiparticles called surface phonon ...

Predicting phonon properties and thermal conductivity requires a calculator that provides the energy of a set of atoms and, ideally, the net force exerted on each atom. Density functional theory is a suitable calculator for this purpose. [33,34] [33]. D.

In summary, we have investigated the impact of doubling the mass of hydrogen (deuteration) on the phonon dispersion and

thermal transport properties of methylammonium lead iodide perovskite....

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#### **First principles study on the structural, electronic and ...**

The entire set of all possible phonons that are described by the phonon dispersion relations combine in what is known as the phonon density of states which determines the heat capacity of a crystal. By the nature of this distribution, the heat capacity is dominated by the high-frequency part of the distribution, while thermal conductivity is primarily the result of the low-frequency region.

#### **Thermal transport properties of GaN with biaxial strain ...**

Thermal properties of graphene and graphite have been investigated by employing the analytical expressions for the phonon dispersion relations and the vibrational density of states derived by Nihira and Iwata, which are based on the semicontinuum model proposed by Komatsu and Nagamiya.

#### **Phonon Dispersion - Articles - Scientific Research Publishing**

Thermal properties of bulk zinc-blende boron arsenide (BAs) were investigated by performing ab initio calculations using both the local density approximation (LDA) and generalized gradient approximation (GGA) for the exchange-correlation potential. Phonon dispersion relations were studied within the framework of density

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**Giant isotope effect on phonon dispersion and thermal ...**

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**Thermal properties in the harmonic approximation – hiPhive ...**

Thermal conductivity  $\kappa$  is defined as the energy transmitted per unit time across unit area per unit temperature gradient. Dependence of  $\kappa$  on  $dT/dx$  implies that the thermal energy transfer is a random process involving scattering – introduces mean free path of phonons in the problem.

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**Phonon and Thermal Properties of Quasi-Two-Dimensional ...**

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**Phonon - Wikipedia**

**Thermal conductivity and phonon hydrodynamics in ...**

**Lecture 13 Phonons: thermal properties**

**nanoHUB-U Thermal Energy at the Nanoscale L3.2: Basic Thermal Properties - Acoustic Phonon Sp. Heat Skoltech Colloquium:**

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**Heat** Phonon Calculations in Materials Science using VASP \u0026

phonopy Near-equilibrium Transport Lecture 9: Phonon Transport

Nanomanufacturing: 06 Thermal properties of nanostructures

Thermal properties of materials *Mod-01 Lec-14 Lattice Vibrations*

*(Continued) Phonon thermal conductivity THERMAL PROPERTIES*

*Thermal conductivity and phonon collisions 172 - Phonons.*

**Phonons at Surfaces (VintageVideo)** *Making sense of Brillouin Zones - Part 1*

*Dynamic Control of Phonon Propagation in*

*Phononic Crystal Waveguide* **PHYS 201 | Dispersion 3 - Reading**

**Dispersion Curves** **Solid State Physics in a Nutshell: Week**

**5.1 Introduction to Phonons** *How to measure heat flux? Thermal*

*Expansion {Texas A\u0026M: Intro to Materials} Electron -*

*Phonon Interaction (Simple)* **Thermal Expansion {Texas**

**A\u0026M: Intro to Materials (MSEN 201)}** **Introduction to**

**Solid State Physics, Lecture 5: One-dimensional models of**

**vibrations in solids** *Phonon thermal transport in 2D materials -*

*LUCAS LINDSAY Solid State Physics in a Nutshell: Topic 6-3: Thermal*

*Conductivity Understanding what is Thermal Conductivity?*

**PHONONS N-PROCESS U-PROCESS (HINDI) lec-25 nano-**

*HUB-U Thermal Energy at the Nanoscale L5.3: Carrier Scattering -*

*Phonon-Phonon Scattering MSN 514 - Lecture 32: Phonons and*

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