

Physics Colloquium

Can the thermal conductivity of semiconductors be controlled by impurities?

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Calculating the vibrational properties of impurities in semiconductors such as Si has kept theorists busy for a few decades. The early focus has been on predicting the frequencies of IR- or Raman-active local vibrational modes. However, the knowledge of the entire dynamical matrix is precious. First, its eigenvalues allow the identification of *all* the impurity-related localized modes in the system. Second, the complete phonon density of states can be obtained. It is needed to calculate the specific heat and vibrational free energy. Third, the eigenvectors of the dynamical matrix can be used to 'prepare' a supercell in thermal equilibrium at any temperature (as long as it is not too high) without the need for any thermalization or even a thermostat. This opens the door to practical non-equilibrium molecular-dynamics simulations with controlled temperature fluctuations. One application involves the temperature-dependence of vibrational lifetimes. Another is the calculation of thermal conductivities as a function of the impurity content of the material.

This talk will begin with a few comments about why manipulating the thermal conductivity of materials is important. Then, I will discuss the existing (empirical) theoretical methods for calculating thermal conductivities, and discuss how we approach this problem with first-principles techniques (for the first time). Preliminary results show that unexpected physics is taking place. Let the funding continue...

**Thursday, September 10, 3:30pm,
SCI 007**

refreshments will be served in Sci 103 at 3:00pm