Phonon calculations: Techniques and applications

By
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Date: 22 April 2015, Wednesday
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Venue: MAS Executive Classroom 1
Host: Prof Shen Zexiang

Abstract
The calculation of the vibrational frequencies of a crystal is important to the understanding of phase stability, phase transitions, thermodynamics, and Raman and infrared spectroscopies of materials. In this talk we will give a brief introduction to phonon calculations. Some existing tools for performing phonon calculations will be presented. Some general guidelines will be given. We will present some illustrative results on Raman spectroscopies, thermal conductance, figures of merits, and thermal expansion coefficients of Bi2S3, Sb2S3, graphene, graphene nanoribbons, and other materials.

Short Biography
Dr. GAN Chee Kwan studied physics and computational science at the National University of Singapore and obtained a B.Sc. degree in 1995.

He then studied the theory of condensed matter at the University of Cambridge, and obtained a Ph.D. degree under the supervision of Prof. Mike Payne in 2001. He spent the next three years at the Los Alamos National Laboratory as a postdoctoral research fellow specializing in the parallelization and application of a density-functional code. He then joined the Institute of High Performance Computing where he is now a Senior Scientist. Dr. Gan’s expertise is in the area of condensed matter physics and high performance computations. He has worked on various methodology developments for high-performance parallel computing. He has developed various codes such a tight-binding code, a phonon code, and a heat transport code based on the nonequilibrium Green’s function method. He has studied the thermodynamic properties of semiconductor alloys, heat transport properties of graphene and thermoelectric materials, and various magnetic materials. His current research interest is to develop methods to calculate thermal properties of materials taking into account various mechanisms such as phonon-phonon scattering, electron-phonon scattering, and interaction of phonons with localized defects. He published in several high impact journals such as Nature Nanotechnology, ACS Nano, Nano Letters, and JACS.