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Phonon spectrum in a CdSe nanowire[1] CHRIS BARRETT, Material Science and Engineering Department, University of California at Berkeley, LIN-WANG WANG, Material Sciences Division — It is important to calculate the phonon spectrum of realistic nanowires, e.g. to understand its thermo conductivity or to calculate the electron-phonon interaction. In this talk, we will present results of phonon spectrum calculation using valence force field (VFF) method. An important issue is to construct the VFF to describe the surface atomic displacement. We have developed a general VFF formalism to fit our VFF result with the density functional theory (DFT) calculated surface atom displacement energies. In particular, the (10-10) CdSe surface is modelled with Cd-Se dimerization. We will discuss the quality of such VFF model. The phonon spectrum of the nanowire will be presented, and its implication on the phonon transport and electron-phonon coupling will also be discussed.

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