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Electron-Phonon Coupling in a CdSe Nanowire[1]
CHRISTOPHER BARRETT, Department of Materials Science & Engineering, UC Berkeley, LIN-WANG WANG, Materials Sciences Division, Lawrence Berkeley National Laboratory — It is important to calculate the coupling between phonons and electrons in realistic nanostructures, e.g. to understand carrier cooling and dynamics in a nanowire. In this talk, we will present results of phonon spectrum calculations using a customized valence force field (VFF) method. This customized VFF method is developed to be fittable to the results of any ab-initio calculations, with density functional theory (DFT) results being used in this work. By fitting many different DFT calculations on different motifs and their perturbations, we have obtained in the custom VFF a very efficient method that closely reproduces DFT phonons for CdSe nanowires with (10-10) surfaces having Cd-Se dimerization. We have also combined the results of these phonon spectrum calculations with electronic structure calculations to obtain the electron-phonon coupling. We will present this result and and show how the electron-phonon coupling affects the carrier dynamics in the nanowire.

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