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Predicting Phononic and Thermal Properties of Nanocrsytal Superlattice Structures Using Atomistic Models MEHDI ZANJANI, JENNIFER LUKES, University of Pennsylvania — We use fully atomistic models with MD simulations to predict phononic and thermal properties of nanocrystal superlattices (NCSLs). NCSLs are formed by assembly of nanocrystals into organized structures with interesting and tunable properties. They present new phononic behaviors by combining dissimilar materials structured on the nanometer scale. The small thermal conductivity of these materials makes them promising candidates for thermoelectric applications as well. We have calculated phonon dispersion curves of NCSLs by generalizing the lattice dynamics methods. We also calculated thermal conductivity of these materials using 3-D equilibrium MD simulations and the Green-Kubo method. Atomistic models along with MD simulations provide a complement to experiments for understanding the behavior of NCSLs, and help us modify the design of these structures to achieve better phononic and thermal properties.

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