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First principles calculations of the interactions of a filling atom with its neighboring atoms in a skutterudite (LaFe4Sb12)[1] JOSEPH FELDMAN, NRL, DAVID SINGH, ORNL, NOAM BERNSTEIN, NRL — The room temperature lattice thermal conductivity of filled skutterudites is about a factor of 5 smaller than that of unfilled skutterudites which has caused a great deal of attention to be focused on these materials from a scientific standpoint, as well as a technological one, i.e., thermoelectric applications. In an effort to gain a microscopic understanding of this we have previously used a central force model and Green-Kubo techniques with force parameters heavily based on first principles results [Bernstein et al., Phys Rev. B **81**, 134301 (2010)]. However, as we had no first principles information on the La-Fe cubic anharmonic parameters in LaFe4Sb12 we have performed new direct method calculations for a larger supercell than the Bravais cell used previously to compute not only the six independent La-Fe cubic anharmonic parameters but numerous other parameters. Atomic forces were computed in various structural configurations differing only by the coordinates of one of the two La positions in the simple cubic supercell. DFT results are compared for LAPW, PAW, and plane-wave pseudopotential methods.

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