Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Green Kubo calculations of thermal conductivity for skutterudites[1] JOSEPH FELDMAN, George Mason University and Center for Computational Materials Science, Naval Research Laboratory, NOAM BERNSTEIN, Center for Computational Materials Science, Naval Research Laboratory, DAVID SINGH, Materials Science and Technology Division, Oak Ridge National Laboratory — The thermal conductivity of skutterudites have been studied experimentally for several years and the results clearly show a strong dependence on whether or not the skutterudite is filled. This result has been explained, and indeed predicted, by the presence of a rattling ion in the filled materials. On the other hand, it has been shown that the potential of the rattling ion is not dramatically anharmonic as expected within a simple rattling ion concept. In this work we will discuss the thermal conductivity of a realistic model of the skutterudites through a Green-Kubo calculation using molecular dynamics. We represent the interatomic potentials as Taylor series in displacements from equilibrium with up to quartic anharmonic terms. In this initial study we explore different central force parameters from empirical models and first principles calculations in the literature.

[1]Work at ORNL funded by DOE EERE

Joseph Feldman
George Mason University and Naval Research Laboratory

Date submitted: 13 Dec 2006 Electronic form version 1.4