Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Modeling correlated motion in thermoelectric skutterudite materials[1] TREVOR KEIBER, FRANK BRIDGES, Univ of California-Santa Cruz, BRIDGES LAB TEAM — Filled skutterudite compounds, LnT_4X_{12} (Ln=rare earth; T=Fe,Ru,Os; X=P,As,Sb), have previously been modeled using a rigid cage approximation for the "rattling" rare earth atom. The large thermal broadening with temperature of the rattler can be fit using an Einstein model. Recent measurements of the second neighbor Ln-T peaks show an unusually large thermal broadening suggesting motion of the cage of atoms. To incorporate these results we developed three and four mass spring models to give the acoustic and optical phonon mode spectra. For the simplest three mass model we identify the low energy optical mode as the rattling mode. This rattling mode is likely coupled to the acoustic mode, and responsible for the low thermal conductivity of the skutterudite compound. We extend this model to four atoms to describe the CuO_4 rings in oxy-skutterudites and the X_4 rings in LnT_4X_{12}. This talk provides a model for the experimental results of the previous presentation.

[1]Support: NSF DMR1005568

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Date submitted: 14 Nov 2013 Electronic form version 1.4