Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Thermal transport properties of complex oxides from first principles AQYAN BHATTI, Univ of Texas, Austin, ANKIT JAIN, ALAN MCGAUGHEY, Carnegie Mellon University, NICOLE BENEDEK, Univ of Texas, Austin — Thermal transport properties of materials are key parameters in the design of many engineering devices. For this reason, it is highly desirable to be able to control or tailor the thermal properties of materials for specific applications. Complex oxides are attractive in this regard, due to their low and potentially highly tunable thermal conductivity. However, the theoretical description of the thermal transport properties of oxides presents a number of challenges compared to conventional semiconductors. For example, oxides tend to have complex crystal structures and the atoms interact through long-range electrostatic forces. In this talk, we use the example of $PbTiO_3$ to discuss some of the challenges and opportunities associated with thermal transport predictions in complex oxides. For example, many oxides contain very low-lying optical branches, which may provide important acoustic-optical scattering channels. In addition, it is often possible to tune the frequencies of such optical modes with epitaxial strain. We also link the observed negative thermal expansion behavior of $PbTiO_3$ to two zone-boundary modes with large, negative Grüneisen parameters and comment on the consequences of this finding for the thermal transport properties of this material.

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Date submitted: 13 Nov 2014 Electronic form version 1.4