Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Understanding the Origins of Large Negative Thermal Expansion in Ferroelectric Perovskites from First Principles[1] ETHAN RITZ, NICOLE BENEDEK, Cornell University — Many of the functional properties of ABO_3 perovskite oxides (for example, ferroelectricity) are strongly linked to particular phonon modes in the material. In addition, in many cases it is possible to formulate simple guidelines or 'rules of thumb' that link crystal structure and chemistry to specific lattice dynamical characteristics. The thermal transport properties of perovskites are thus potentially highly tunable and dynamically controllable with external fields. We use first-principles density functional theory to reveal new details related to the origin of the large negative thermal expansion (NTE) observed for ferroelectric $PbTiO_3$. Although the origin of NTE in this material is often ascribed to ferroelectricity (which arises from the freezing in of a soft, zone-center optical phonon), our results suggest that zone-boundary modes play a major role in driving NTE. In addition, hybridization between different electronic states has a significant effect on the lattice dynamics of $PbTiO_3$ in general, and its NTE behavior in particular. Our work has implications for the understanding of, discovery and design of NTE in perovskites and other families of inorganic materials.

[1]This work was supported in part by a NASA Space Technology Research Fellowship.

Ethan Ritz
Cornell University

Date submitted: 11 Nov 2016 Electronic form version 1.4