Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Controlling Elastic Properties in Perovskites with Polyhedral Connectivity NICHOLAS WAGNER, JAMES RONDINELLI, Northwestern University — Using density functional theory, we investigate the effect of BO_6 octahedral face-sharing on the macroscopic mechanical properties of ABO_3 compounds (A=Sr, Ba) (B= Ti, Mn, Ni, Zr). We consider four structure prototypes of which three are hexagonal perovskites, exhibiting different ratios of corner-connected octahedra to face-connected octahedra (33%, 50%, & 100%). The fourth structure, cubic perovskite, exclusively exhibits corner-connected octahedra. We find that increasing the proportion of face-sharing to corner-sharing results in a decrease in the elastic constants independent of the d orbital filling or cation size. Next, we explore the role of local and crystal structure features on this trend with a random forest regression model to identify that the volume per atom and trigonal distortion amplitude may serve as useful descriptors to predict this decrease. Finally, we propose how changing this trigonal distortion can potentially be used to engineer electronic properties such as the bandgap in these materials.

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Date submitted: 31 Oct 2016 Electronic form version 1.4