Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Searching for ferroelectricity and piezoelectricity in Heusler compounds using first-principles calculations ANINDYA ROY, JOSEPH BENNETT, KARIN M. RABE, DAVID VANDERBILT, Rutgers University — Hundreds of half Heusler (HH) and full Heusler (FH) compounds have been synthesized, and they exhibit a multitude of properties. However, we are unaware of any Heusler compounds showing ferroelectricity (FE), or for which the piezoelectricity (PzE) has been measured. Determining these polar properties would be of theoretical interest as well as having practical importance for the design of new functional materials. In this *ab initio* study, we search a large set of HH and FH compounds, both known and hypothetical, for FE/PzE. We screen the zone-center phonons, computed with first-principles density-functional-theory methods, for unstable polar modes that would drive a distortion to a ferroelectric phase, and calculate PzE coefficients of compounds in the $F\bar{4}3m$ space group, which includes all HH and many FH, using density-functional perturbation theory. Preliminary results from our calculations confirm that the Heusler compounds are very robust against FE instabilities. However, we found several HH compounds having e_{14} coefficients in the range of 0.5-1.0 C/m^2, comparable to that of some well-known piezoelectric materials such as ZnO. We also investigate the effects of epitaxial constraints on these properties, both for bulk materials and for superlattices built of Heusler materials.

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Date submitted: 23 Nov 2010 Electronic form version 1.4