Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Search for New High Performance Piezoelectrics P. GANESH, RONALD E. COHEN, Carnegie Institution of Washington — In an effort to design new high performance piezoelectric materials, we have performed first-principles calculations to study the energetics of several ABO_3 type materials, with the 'A' site being occupied by two types of atoms. The motivation comes from recent findings of a morphotropic-phase boundary, which gives rise to large electromechanical coupling, at high pressure and low temperatures in pure $PbTiO_3$[1]. This prompted us to substitute the 'A' site with a smaller atom compared to Pb to apply "chemical pressure" and tune the morphotropic-phase boundary to lower pressures. We have discovered $(Pb_{1/2}\ Sn_{1/2})TiO_3$, $(Pb_{1/2}\ Ge_{1/2})TiO_3$ and $(Sn_{1/2}\ Ge_{1/2})TiO_3$ to be promising new piezoelectric materials. $(Pb_{1/2}\ Sn_{1/2})TiO_3$ shows lower energy monoclinic phases (space groups Cm with polarization along [xxz] and Pm with polarization along [x0z]) compared to the layered tetragonal phase (space group P4mm with polarization along [001]) while the remaining two compounds have a rhombohedral (space group R3m with polarization along [111]) ground-state compared to the tetragonal phase in the rock-salt pattern (space group I4mm with polarization along [001]). Our results also suggest ease of polarization rotation and large electromechanical strain. [1] Zhigang Wu and Ronald E. Cohen, PRL, **95**, 037601, 2005

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Date submitted: 30 Nov 2007 Electronic form version 1.4