Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

**Why isn't $CsSnF_3$ ferroelectric?** EVA H. SMITH, School of Applied and Engineering Physics, Cornell University, NICOLE A. BENEDEK, Materials Science and Engineering Program, The University of Texas at Austin, CRAIG J. FENNIE, School of Applied and Engineering Physics, Cornell University — Complex fluorides are an interesting class of materials to explore for new ferroelectrics and multiferroics. The elucidation of design rules for new ferroelectric fluorides is challenging because polar fluorides tend to form in structures with a large number of atoms in the unit cell and the ferroelectricity is almost always of the geometric type. In this talk we will discuss our recent attempt to rationally design new polar fluorides from first principles. By exploring the relative stability of the subgroups of the perovskite manifold (using the phonons of the 5-atom cubic structure as a guide), we reveal the origin of ferroelectricity in R3c $CsPbF_3$, the only known polar $ABF_3$ compound. Comparison with $CsSrF_3$, which has a similar tolerance factor but no lone pair cation, reveals that the interplay between lone-pair localization and rotations stabilizes the rotation pattern most compatible with ferroelectricity, *i.e.*, $a^-a^-a^-$, rather than the more common $a^-a^-c^+$. Next we replace $Pb^{2+}$ with another lone pair cation, $Sn^{2+}$. Within a perovskite manifold of states $CsSnF_3$ is ferroelectric, yet synthesis of this compound by our experimental collaborators shows that not only isn't it ferroelectric, it isn't even a perovskite. Why?

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Date submitted: 09 Nov 2012 Electronic form version 1.4