Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

New design strategy for realizing multiferroic materials DANILO PUGGIONI, Department of Materials Science and Engineering, Northwestern University, Evanston, IL60208, USA, GIANLUCA GIOVANNETTI, MASSIMO CAPONE, CNR-IOM-Democritos National Simulation Centre and International School for Advanced Studies (SISSA), Via Bonomea 265, I-34136, Trieste, Italy, JAMES RONDINELLI, Department of Materials Science and Engineering, Northwestern University, Evanston, IL60208, USA — Ferroelectricity is a property that only insulating materials can exhibit. For this reason, nearly all searches for new multiferroic compounds, those simultaneously exhibiting ferroelectric and magnetic order, have focused on *insulating* magnetic oxides. Here, we propose a different approach: Start from a *conducting* oxide with broken inversion symmetry and search for routes to induce long-range magnetic order [1]. Using density-functional and dynamical mean-field theories, we investigate the electronic properties of the polar metallic oxide $LiOsO_3$. We show that a multiferroic state can be engineered by enclosing $LiOsO_3$ between an insulating material, $LiNbO_3$. We predict that the 1/1 superlattice of $LiOsO_3$ and $LiNbO_3$ exhibits strong coupling between magnetic and ferroelectric degrees of freedom with a ferroelectric polarization of 41.2 μCcm^{-2}, Curie temperature of 927 K, and Néel temperature of 379 K. Our results show that one can start with polar metallic oxides to make multiferroics.

[1] D. Puggioni *et al*, Phys. Rev. Lett. **115**, 087202 (2015).

Danilo Puggioni
Department of Materials Science and Engineering, Northwestern University, Evanston, IL60208, USA

Date submitted: 04 Nov 2015 Electronic form version 1.4