Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Epitaxial strain effects on layered polar oxides from first-principles XUEZENG LU, JAMES RONDINELLI, Department of Materials Science and Engineering, Northwestern University, MATERIALS THEORY AND DESIGN GROUP TEAM — Epitaxial strain is a powerful tool to generate ferroelectric phases in thin films owing to polarization-strain coupling. The coupling of the oxygen rotations to strain can also be exploited to realize oxygen rotation-sensitive properties such as metal-insulator transitions and magnetic reconstructions. Here, we use electronic structure calculations to investigate the effects of biaxial strain on (001) thin films of the hybrid-improper ferroelectric $Ca_3Ti_2O_7$. Besides the bulk $Cmc2_1$ phase, we also find a new phase emerges under both experimentally accessible biaxial compressive and tensile strains. Furthermore, a large change in the dielectric anisotropy of the film is found at the tensile phase boundary, which we propose could be electric field tunable. Our results may offer a route to search for new functionalities in layered-perovskite oxides.

Xuezeng Lu
Department of Materials Science and Engineering, Northwestern University

Date submitted: 05 Nov 2015 Electronic form version 1.4