

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

First principles study of piezorotation in thin-film LaAlO₃ ALISON HATT, NICOLA SPALDIN, University of California, Santa Barbara — We investigate the effect of biaxial strain on [001] thin-film LaAlO₃ using density functional calculations. We find that the essentially rigid rotations of the AlO₆ octahedra vary linearly with strain, a phenomenon which may be described as piezorotation by analogy with piezomagnetism or piezoelectricity [S. Denev, et al., Phys. Rev. Lett. 100, 257601 (2008).] Within a small range of experimentally achievable strain values, we find that epitaxial strain can stabilize several distinct modes of cooperative rotations not found in the bulk, and identify first order phase transitions between states with different piezorotative responses. Finally, we investigate how the electronic and elastic properties are affected by proximity to the strain-induced phase transitions.

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Date submitted: 19 Nov 2008

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