Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

The Effect of Biaxial Strain and Layer Thickness on Octahedral Rotation in $LaNiO_3$[1] PATRICK MCBRIDE, ANDERSON JANOTTI, CYRUS DREYER, BURAK HIMMETOGLU, CHRIS VAN DE WALLE, Univ of California - Santa Barbara — Heterostructures of complex oxides have attracted great attention for the interplay between structure, electronic, and magnetic properties, offering unique opportunities in device applications. Here we investigate the effects of epitaxial strain and layer thickness on the structural properties of $LaNiO_3$. We perform first-principles calculations based on density functional theory to investigate the NiO_6 octahedral tilts and Ni-O bond lengths of biaxially stressed $LaNiO_3$ layers in $LaNiO_3/SrTiO_3$ superlattices. Recent experimental results suggest that octahedral connectivity in these superlattices strongly influence the octahedral rotations in the $LaNiO_3$ layer, and thus, determines its electronic behavior. In this talk we will present a quantitative analysis for the octahedral tilt angles as a function of both biaxial stress and distance from the substrate for $LaNiO_3$ grown on $SrTiO_3$ (001). Our results indicate that $LaNiO_3$ exhibits vanishing octahedral tilt angles under certain strain conditions, a finding that holds important consequences for its electronic properties.

[1]Supported by the Bonderson Foundation and the National Energy Research Scientific Computing Center

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Date submitted: 08 Jan 2014 Electronic form version 1.4