# *Ab initio* demonstration of structural phase transitions in Ruddlesden-Popper phases of strontium titanate

Jeehye Lee and Tomas A. Arias
*Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, New York 14853*
(Dated: May 24, 2010)

We present the first systematic *ab initio* study of octahedral rotations in Ruddlesden Popper (RP) phases of strontium titanate, $Sr_{1+n}Ti_nO_{3n+1}$, as a function of epitaxial strain and phase number $n$. We find the novel behavior that, contrary to the bulk parent material $SrTiO_3$ and previous theoretic studies which did not explore the influence of strain, under expitaxial compression, the RP phases exhibit a non-ferroeletric antiferrodistortive (AFD) rotational phase with a rich structure over a significant range of strains before the ferroelectric instability. Focusing in this non-ferroelectric phase, we demonstrate how the bulk behavior recovers smoothly as $n$ increases and introduce a simple model Hamiltonian consistent with our results that shows that the critical strain for the onset of this non-ferroelectric AFD phase scales as $1/n^2$. We also report the substantial out-of-plane lattice expansion, which can be observed in experiments as a signature for the AFD transition.