

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Ab-initio investigation of the octahedra rotation in strained Ruddlesden-Popper(RP) phases¹ JEEHYE LEE, TOMAS ARIAS, Laboratory of Atomic and Solid State Physics, Cornell University — This talk presents the result of an ab-initio study of Ruddlesden-Popper(RP) phases for $Sr_{n+1}Ti_nO_{3n+1}$ ($n = 1, 2, 3, \infty$) compounds with the density functional theory(DFT). In particular, we present results for the relation between octahedral rotations and external strains. We find that rotational reconstructions are energetically favorable under nonzero in-plane strains with a critical strain that depends on both n and rotational configurations. We also explore the relative stability of RP phases with different values of n under epitaxial conditions.

¹This work was supported by the Cornell Center for Materials Research (CCMR), a Materials Research Science and Engineering Center of the National Science Foundation(DMR 0520404).

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Date submitted: 20 Nov 2009

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