

Abstract Submitted
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Strain Control of Electronic Phase in Rare Earth Nickelates¹

ZHUORAN HE, ANDREW MILLIS, Dept. of Physics, Columbia Univ. — In this work, we use DFT+ U methods to study the effects of strain on the electronic states and lattice structure of thin films of LuNiO₃. We model the effects of a substrate-induced strain by fixing the in-plane lattice parameter and relax both the c -axis lattice parameter and all internal coordinates. Both compressive and tensile strain destroy the charge order and create a metallic state. Tensile strain induces a staggered Jahn-Teller order. The staggered Jahn-Teller state is shown to compete with the charge-ordered state. The transitions are found to be first order, but the insulating gap in the charge-ordered phase varies substantially with applied strain. Implications for experiments are discussed.

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