Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Jahn-Teller physics and orbital control in oxide heterostructures: a first-principles study of $LaNiO_3/LaXO_3$ (X= B, Al, Ga, In)[1] MYUNG JOON HAN, Physics, Columbia University, CHRIS A. MARIANETTI, Applied Physics and Applied Mathematics, Columbia University, ANDREW J. MILLIS, Physics, Columbia University — Generalized Gradient Approximation (GGA) density functional calculations are used to show that different choices of spacer layer $LaXO_3$ in $LaNiO_3/LaXO_3$ heterostructures lead to different relative occupancies of Ni $3z^2-r^2$ and x^2-y^2 orbitals, with the sign of the orbital polarization even reversing as the B-site atom in the spacer layer is changed from $X = B$ through Al, Ga to In. The crucial role played by the hybridization of the apical oxygen to the spacer layer ($LaXO_3$) is demonstrated. Extensions to other systems and implications for many-body calculations are discussed.

[1]This research was supported by the Army Research Office under contract W911NF0910345

Myung Joon Han
Physics, Columbia University

Date submitted: 19 Nov 2009 Electronic form version 1.4