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.

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