Abstract Submitted
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**Ionic Potential and Band Narrowing as a Source of Orbital Polarization in Nickelate/Insulator Superlattices**[1] ALEXANDRU B. GEORGESCU, Department of Physics, Yale University, ANKIT S. DISA, DIVINE P. KUMAH, SOHRAB ISMAIL-BEIGI, FREDERICK J. WALKER, CHARLES H. AHN, Department of Applied Physics, Yale University — Nickelate interfaces display complex, interacting electronic properties such as thickness dependent metal-insulator transitions. One large body of effort involving nickelates has aimed to split the energies of the Ni 3d orbitals (orbital polarization) to make the resulting band structure resemble that of cuprate superconductors. The most commonly studied interfacial system involves superlattices of alternating nickelate and insulating perovksite-structure layers; the resulting orbital polarization at the nickelate-insulator interface is understood as being due to confinement or structural symmetry breaking. By using first principles theory on the $NdNiO_3/NdAlO_3$ superlattice, we show that another important source of orbital polarization stems from electrostatic effects: the more ionic nature of the cations in the insulator (when compared to the nickelate) can shift the relative orbital energies of the Ni. We use density functional theory (DFT) and add electronic correlations via slave-bosons to describe the effect of correlation-induced band narrowing on the orbital polarization.

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