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A structural route to tuning the orbital structure of nickelates DIVINE KUMAH, ANKIT DISA, ANDREI MALASHEVICH, HANGHUI CHEN, SOHRAB ISMAIL-BEIGI, FRED WALKER, CHARLES AHN, Center for Research on Interface Structures and Phenomena (CRISP), Yale University and Department of Applied Physics, Yale University — The rare-earth nickelates display a range of interesting magnetic and electronic phenomena arising from the strong coupling of the atomic-scale structural properties of these systems to the charge and orbital degrees of freedom. We report on modifying the orbital polarization in nickelate based heterostructures, motivated by the goal of emulating high-Tc cuprate behavior in the nickelates. Using a combination of synchrotron diffraction structural and spectroscopic characterization and first principles theory, we show how the design of a structure that splits the relative electronic occupation of Ni d x^2-y^2 and Ni d $3z^2$-r^2 orbitals, is achieved in three-component heterostructures. These structures are comprised of $LaTiO_3$/$LaNiO_3$/$LaAlO_3$ and are grown using molecular beam epitaxy. The key features of the theoretically proposed structure, including an internal polar field, a electron transfer from Ti to Ni, and a orbital polarization of the Ni-eg states, are experimentally studied.

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