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Engineering orbital polarization in three-component nickelate heterostructures

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The interplay between the structural and physical properties of transition metal complex oxides allows for the engineering of their functional properties by tuning atomic-scale structure using interfacial coupling. We show how this principle can be used to achieve orbital polarization and two-dimensional electronic conductivity in nickelate heterostructures [1, 2]. Using a combination of first principles theory and synchrotron-based experiments, we identify key structural features in LaNiO3 thin films grown using molecular beam epitaxy, allowing one to correlate differences in physical structure with electronic transport properties and x-ray absorption spectroscopy measurements. By applying general design principles, such as charge transfer and inversion symmetry breaking, which lead to degeneracy breaking of the Ni 3d orbitals, one can design and fabricate tri-component superlattices to engineer the electronic and orbital properties of rare-earth nickelate compounds, achieving a two-dimensional single band electronic surface at the Fermi energy.

[1] H. Chen et. al. Phys. Rev. Lett. 110, 186402 (2013)
[2] D. Kumah et. al. Adv. Materials 26, 1935 (2014)