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Field-effect modulation of structure and carrier transport of $LaNiO_3$ thin films ANDREI MALASHEVICH, MATTHEW S.J. MARSHALL, ANKIT S. DISA, FREDERICK J. WALKER, CHARLES H. AHN, SOHRAB ISMAIL-BEIGI, Center for Research on Interface Structures and Phenomena and Department of Applied Physics, Yale University — Materials exhibiting large changes in resistivity in response to applied electric fields are of importance due to their technological applicability, e.g., in field-effect transistors. Of particular interest are thin film oxide/ferroelectric interfaces: the ferroelectric permits dynamic modulation of electronic transport in the oxide film which is crucial for non-volatile memory applications. In the standard field effect, resistance modulations result from changes in carrier density created by the applied electric field. At ferroelectric interfaces, however, other mechanisms can come into play. Our experiments show that at the (001) interface of rare-earth nickelates and ferroelectric $Pb_{0.8}Zr_{0.2}TiO_3$ (PZT), the change of carrier mobility plays a critical role in the electronic transport. Here, we present a first-principles study of the interface between a thin film of conducting $LaNiO_3$ and ferroelectric $PbTiO_3$ (PTO). We analyze the dependence of the atomic structure of the interface on the PTO polarization and the effect of the structural changes on the electronic bands and associated carrier transport. We also describe the methodological challenges in transport calculations of metal/ferroelectric interfaces and some ways to address them.

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