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The effect of the interface termination on the atomic and electronic structure of $LaNiO_3/PbZr_xTi_{1-x}O_3$[1] 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 — Thin film metal oxide/ferroelectric interfaces can exhibit dependence of conductivity on the polar state of the ferroelectric layer. This property has potential for technological applications in non-volatile field-effect devices. Recently, we demonstrated that ferroelectric $PbZr_{0.2}Ti_{0.8}O_3$ (PZT) can be used to modulate conductivity of the (001)-oriented $LaNiO_3$/PZT interface. We found that changes in conductivity result primarily from large mobility changes in the interfacial channel region. In this study, we investigate the effect of the $LaNiO_3$ film termination (LaO vs NiO_2) on the atomic structure and electronic properties of $LaNiO_3$/PZT. We present the results of the first-principles calculations of the atomic structure of the related $LaNiO_3/PbTiO_3$ interface for both $LaNiO_3$ terminations. For each termination, we analyze the dependence of the atomic structure and electronic properties on the ferroelectric $PbTiO_3$ polar state and compare the results to available experimental observations.

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