The effect of the interface termination on the atomic and electronic structure of LaNiO$_3$/PbZr$_x$Ti$_{1-x}$O$_3$ ANDREI MALASHEVICH, MATTHEW S. J. MARSHALL, ANKIT S. DISA, FREDERICK J. WALKER, CHARLES H. AHN, SOHRAB ISMAIL-BEI GI, 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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