MAR15-2014-020566

Abstract for an Invited Paper
for the MAR15 Meeting of
the American Physical Society

Interrelation of polarity, screening, structure, and electronic states at nickelate interfaces[1]

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A basic property of metal oxides is ionicity: the metal (cation) and oxygen (anion) sites have different electron densities and thus different charge states. This then permits the existence of polarity whether (1) in static form deriving from the choice of the terminating atomic plane at an interface, or (2) in dynamic form through the existence of ferroelectricity which permits switching of the polarity at an interface. The polarity drives the accumulation of charge, modification of the atomic-scale structure, and alteration of the electronic states at an interface. Here we describe an interconnected body of recent collaborative work on nickelate interfaces where electronic transport is strongly modified by the choice of polarity and/or ferroelectric polarization [1,2,3]. Combining first principles theory and experiments allows one to unravel the microscopic origin of the interfacial phenomena. In the case of ultrathin $LaNiO_3$ films, there is a strong dependence of transport properties on the choice of surface termination and the resulting near-surface structural distortions, all of which take place within the screening length of the nickelate. In the case of $LaNiO_3/Pb(Zr_xTi_{1-x})O_3$ interfaces, we show that the striking dependence of measured transport properties on the ferroelectric polarization is based on a change of mobility, as opposed to carrier density, at the interface that derives from the creation of a new conducting channel in the (nominally insulating) interfacial region of the ferroelectric.

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[2] D. P. Kumah, A. Malashevich, A. S. Disa, D. A. Arena, F. J. Walker, S. Ismail-Beigi, and C. H. Ahn, "Effect of Surface Termination on the Electronic Properties of LaNiO3 Films," Phys. Rev. Applied, vol. 2, 054004 (2014).

[3] M. S. J. Marshall, A. Malashevich, A. S. Disa, M.-G. Han, H. Chen, Y. Zhu, S. Ismail-Beigi, F. J. Walker, and C. H. Ahn, "Conduction at a Ferroelectric Interface," Phys. Rev. Applied, vol. 2, 051001 (2014).

[1]Primary support for this work is provided by the NSF via grant MRSEC DMR-1119826.