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**Role of polarization screening and oxygen vacancy in LaAlO<sub>3</sub> overlayer on SrTiO<sub>3</sub> (001)** YUN LI, JAEJUN YU, Seoul National University, Seoul, Korea — The observation of a high mobility electron gas in the *n*-type (LaO)/(TiO<sub>2</sub>) interface between two band-gap insulators LaAlO<sub>3</sub> (LAO) and SrTiO<sub>3</sub> (STO) has generated intense research activities. We investigate the role of polarization screening and oxygen vacancy in determining induced carrier density at the *n*-type interface of LAO overlayer on STO by carrying out density-functional-theory calculations. When no oxygen vacancy is present, the detailed balance between the lattice polarization and the charge transfer is found to be crucial for the carrier at the *n*-type interface of LAO overlayers on STO(001). When the LAO overlayers are over a critical thickness, the charge transfer from the LAO surface to the interface is compensated by the electrostatic screening due to the polarization distortions across the LAO layers. To identify the role of oxygen vacancy, we calculated the electronic structure and formation energy of the oxygen vacancy at various locations. The potential screening and induced carrier are strongly affected by the vacancy density. We discuss the mechanism of carrier generation by the oxygen vacancy at the interface.

Jaejun Yu  
Seoul National University

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