Structural and electronic properties of heterointerfaces composed of ferroelectric oxides

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For the paradigmatic oxide heterostructure with $LaAlO_3$ (LAO) thin films grown on $SrTiO_3$ (STO) substrates, distinct electronic phases have been extensively characterized at the LAO/STO interface: for LAO films with more than three layers and LaO termination towards the TiO_2 interface, a two dimensional electronic system (2DES) is formed in the STO layers next to the interface which becomes superconducting below a temperature below 300 mK [1, 2]. Remarkably, the superconducting state coexists with a magnetic state being stable up to the room temperature. It was concluded, that the primary mechanism responsible for the 2DES formation is electronic reconstruction.

Analogous to the ionic polar discontinuity, the 2DES may be created at an interface due to electric polarization discontinuity [3,4]. An attractive materials for such purpose are ferroelectrics. They have a wide range of different distinctive properties, among them: spontaneous polarization switching, high dielectric permeability, dielectric nonlinearity, piezo- and pyro- activity, linear and quadratic electro-optical effects. Such a functionality can expand the scope of application in nanoelectronics.

In the present work based on first-principles band structure calculations, we demonstrate the possibility of a 2DES formation at the interface composed of perovskite ferroelectric ($KNbO_3$, $BaTiO_3$, $LiNbO_3$, $PbTiO_3$) and a wide band-gap insulator (STO, MgO). We analyze an impact of ferroelectric polarization onto the 2DES conducting properties, as well as a possibility of switchable and controllable metal-insulator transition in considered types of heterostructures.

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[1]. Ohtomo, A. and H. Hwang, “A high-mobility electron gas at the $LaAlO_3/SrTiO_3$ heterointerface,” Nature, Vol. 427, No. 6973, 423-426, 2004.
[2]. N. Reyren, S. Thiel, A. Caviglia et al., “Superconducting Interfaces Between Insulating Oxides,” Science, Vol. 317, No. 5842, 1196–1199, 2007.
[3]. Niranjan, M. K., Y. Wang, S. S. Jaswal, and E. Y. Tsymbal, “Prediction of a Switchable Two-Dimensional Electron Gas at Ferroelectric Oxide Interfaces,” Phys.Rev.L., Vol. 103, No. 016804, 2009.
[4]. Liu, X., E.Y. Tsymbal, and K. M. Rabe, “Polarization-controlled modulation doping of a ferroelectric from first principles,” Phys.Rev.B. Vol. 97, No. 094107, 2018.