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Structural and electronic properties of heterointerfaces composed of complex ferroelectric oxides

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In 2004 the astounding phenomenon was found at the interface between two nonmagnetic wide-band-gap insulative oxides $LaAlO_3$ (LAO) and $SrTiO_3$ (STO) [1]. A two-dimensional electronic system (2DES) is formed in the STO layers next to the interface which becomes superconducting below a temperature of 300 mK [1,2]. Remarkably, this 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 the electronic reconstruction followed by structural reconstruction.

Since then 2DES has been later found in other non-magnetic dielectrics. And all of them have in common is that the creation of 2DES is due to either the polar nature of one of components or due to defects of dopants. Latter, it has been shown that 2DES can be created at the interface of nonpolar oxides one of which is ferroelectric [3,4]. The main advantage of using ferroelectrics is a possibility to switch on and off the polarization and thus to control properties of the electron system.

In the present work based on first-principles band structure calculations, we theoretically investigate the interface between a ferroelectric film ($KNbO_3$, $BaTiO_3$, $LiNbO_3$, $PbTiO_3$) and a nonpolar insulating $SrTiO_3$ (and MgO) substrate. We demonstrate the possibility of a 2DES formation at the interface. 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. We present comparative study of different combinations of components containing varying number of ferroelectric overlayers, as well as layer-resolved density of states.

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