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Structural, electronic and optical properties of heterointerfaces based on antiferromagnet $LaMnO_3$ and ferroelectrics isostructural to $BaTiO_3$

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The astounding phenomenon was found at the interface between two nonmagnetic wide-band-gap insulative oxides $LaAlO_3$ (LAO) and $SrTiO_3$ (STO) in 2004 [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.

One of the most important feature related to the 2DEG formation is the local polarity of layers inside the LAO slab. In the present work we have chosen the $BaTiO_3/LaMnO_3$ (BTO/LMO) heterostructure, where all layers in the simple electronic limit are neutral, but there is a ferroelectric polarization due to the Ti atoms displacements out of octahedron center in the BTO. The direction of such a polarization might be switched by an external electric field. Based on first-principles band structure calculations, we demonstrate the possibility of q-2DES (quasi-two-dimensoinal electron system) formation at the interface composed of perovskite ferroelectric BTO and antiferromagnet manganite LMO. We present the results of structural, electronic and optical properties calculations of BTO/LMO heterostructure composed of varying number of layers. We analyze an impact of ferroelectric polarization onto the q-2DES conducting properties by layer-resolved density of states calculations. Experimental results of optical investigation of $Ba_{0.8}Sr_{0.2}TiO_3/LaMnO_3$ heterostructure are also presented.

The reported study was funded by Russian Scientific Foundation according to the research project No. 18-12-00260.

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