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Structural, electronic and magnetic properties of ferroelectric/dielectric heterostructures

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A quasi-two dimensional electronic system (q2DES) was found at the interface between two nonmagnetic wide-band gap insulating oxides $LaAlO_3$ (LAO) and $SrTiO_3$ (STO) in 2004 [1]. This astounding phenomenon is formed in the STO layers next to the interface. That state becomes superconducting below a temperature of 300 mK [2]. It was concluded, that the primary mechanism responsible for the q2DES formation is the electronic reconstruction followed by structural reconstruction.

Since then q2DES has been later found in other non-magnetic dielectrics. And all of them have in common that the creation of 2DES is due to either the polar nature of one of components or due to defects or dopants. It has been shown that q2DES 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 features 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) and $BaTiO_3/La_2CuO_4$ (BTO/LCO) heterostructures, 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 q2DES formation at the interface composed of perovskite ferroelectric BTO and antiferromagnet manganite LMO or cuprate LCO. We present the results of structural, electronic and optical properties calculations of BTO/LMO and BTO/LCO heterostructures composed of varying number of layers. We analyze a magnetic properties and an impact of ferroelectric polarization onto the q2DES conducting properties by layer-resolved density of states calculations. Experimental results of magnetic field effect on $Ba_{0.8}Sr_{0.2}TiO_3/LaMnO_3$ heterostructure and of the superconducting state of $BaTiO_3/La_2CuO_4$ heterostructure are also discussed.

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