P95

Ab initio insight into the electronic properties of heterointerfaces composed of nonpolar ferroelectric oxides

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Recently, using ab initio calculations it has been predicted that quasi two-dimensional electron system (q2DES) can be created at the interface of nonpolar oxides one of which is ferroelectric [1, 2]. In this case ferroelectric component of the heterostructure causes the electric polarization discontinuity, which leads to the electron transfer from the surface to the interface. Ferroelectrics have a wide range of different distinctive properties which can expand the scope of application in nanoelectronics, among them: spontaneous polarization switching, high dielectric permeability, dielectric nonlinearity, piezo- and pyro- activity, linear and quadratic electro-optical effects.

In the present work *ab initio* investigations were performed for a $LaAlO_3/SrTiO_3$ heterostructure. We used DFT [3] implemented into the VASP program [4]. We performed method approbation [5], investigated necessary conditions for a q2DES formation, analyzed an impact of oxygen vacancies and hydrogen dopants onto the electronic, structural and magnetic properties [6]. We found that four $LaAlO_3$ overlayers are required for conductivity at the interface induction. In the case of $3LaAlO_3/SrTiO_3$ heterostructure conductivity can be induced by defects (oxygen vacancies or hydrogen dopants) located at the surface or at the interface [6].

Approved method and parameters were used for the modelling of heterointerface composed of ferroelectric oxides. We performed comparative analysis of structural and conductive properties of $LaAlO_3/SrTiO_3$ and $LaAlO_3/BaTiO_3$ heterointerfaces, containing polar $LaAlO_3$. Both heterostructures exhibit similar electronic properties with conductive electrons confined within the TiO_2 layer. We investigated ferroelectric polarization impact onto the conductive properties of the nonpolar $BaTiO_3/SrTiO_3$ heterostructure. We found that polarization towards the interface induce conductivity. After that other pairs of ferroelectric/dielectric were investigated: $LiNbO_3/SrTiO_3$ and $PbTiO_3/SrTiO_3$.

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