

Electronic Structure Analysis of Heterointerfaces Based on LaAlO₃ and SrTiO₃

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Since the discovery of high temperature superconductivity a great effort has been made to study the behavior of strongly correlated electrons in transition metal oxides. Various types of the impurities, crystal structure defects, stoichiometry variations, external electric and magnetic fields, light illumination, uniaxial or hydrostatic pressure can serve as the way of control the transition metal oxide properties. Such a variability of the transition metal oxides with respect to different perturbations obviously provides one with a possibility of the "new state engineering" - fine multidimensional tuning to the phenomena predicted by theory. As a result of structural tuning during the heterointerface growing a variety of outstanding many-body phenomena could be observed. Most of the efforts have concentrated on the study of the high-mobility 2D electron gas appearing in heterostructures combining two band insulators. The most studied combination is two band insulators LaAlO₃ and SrTiO₃ (LAO/STO). In 2004 Ohtomo and others found conductivity in this heterointerface [1].

In the present work the electronic properties of heterointerface based on two insulator LAO/STO have been investigated by means of ab-initio calculations within the density functional theory (DFT) [2], implemented into MedeA-VASP 5.3 [3] program. The exchange-correlation functional was considered at the level of the generalized gradient approximation (GGA) [5]. Considered structures consisted of central region of SrTiO₃ (5.5 layers) bounded on both sides with varying layers of LaAlO₃. Two types of contact have been considered (n-type with TiO₂ – (LaO)⁺ layers in the interface and p-type with SrO – (AlO₂)⁻ layers). It was shown that there is a dependence of band-gap on the number of LAO layers. Obtained results agree well with previously available experimental and theoretical data [1, 5, 6]. Also, we have identified the layers which demonstrate non-zero density of states on the Fermi level. Further, the effect of oxygen vacancies on conductivity in the heterointerface will be analyzed.

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