Heterostructures composed of TMO: *ab initio* investigation

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The discovery of two-dimensional electron gas in 2004 by Ohtomo and Hwang [1] boosted a new area of condensed matter physics, when it became possible to combine incompatible properties in one material, for instance, superconductivity and magnetism at the $LaAlO_3/SrTiO_3$ (LAO/STO) interface [2-4].

This area of perovskite based heterostructures were widely investigated revealing a range of outstanding properties. And all of them have in common is that conductivity occurs due to either the polar nature of one of components or due to defects. Later, it has been shown that 2DEG can be created at the interface of nonpolar oxides one of which is ferroelectric [5,6]. 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. Moreover, ferroelectrics have a range of other outstanding properties which might expand the scope of applications in nanoscale electronic devices: there are spontaneous polarization switching, high dielectric permeability, dielectric nonlinearity, piezo- and pyro- activity, linear and quadratic electro-optical effects.

There are a few systems studied by us in this frame: (1) the pattern LAO/STO heterostructure, (2) structures with antiferromagnet and ferroelectric as components, i.e., $LaMnO_3/BaTiO_3$, (3) ferroelectrics with high-temperature superconductors $La_2CuO_4/BaTiO_3$, (4) ferroelectrics on silicon.

(1) For the LAO/STO system by means of *ab-initio* calculations within GGA+*U* approach we performed a systematic variation of the values of the Coulomb parameters applied to the Ti 3*d* and La 4*f* orbitals [7]. We put previous suggestions to include a large value for the La 4*f* states into perspective in order to shift levels to the higher energy and avoid spurious mixing of La 5*d* and 4*f* states. In addition, we identify important correlations between the local Coulomb interaction within the La 4*f* shell, the band gap, and the atomic displacements at the interface. We demonstrated [8] an impact of electron-donor defects (H-adatom, O-vacancy and also H-adatom+O-vacancy) in different concentration and located in different layers of LAO and STO slabs separately and in the heterostructure on the structural and electronic properties. We have shown that surface defects (oxygen vacancies and hydrogen adatoms) shift the Fermi-level to the higher energy, which leads to an insulator-metal transition in a STO slab and in the LAO/STO heterostructure with three LAO overlayers, whereas a LAO slab undergoes a transition from semiconductor to insulator state. We addressed the defect profiles through the entire heterostructure and reconsider orbital reconstruction of the Ti 3*d* states.

(2) For the $LaMnO_3/BaTiO_3$ (LMO/BTO) system we have demonstrated that a spin-polarized 2DEG occurs without imposed polarization, localized mainly in the MnO layers with a maximum at the interface [9]. Therefore, the coexistence of magnetism in a 2DEG, i.e., a spin-polarized 2DEG, is presented in the LMO/BTO heterointerface. Arising conducting state occurs due to the structural deformations primarily within the interfacial TiO_2 layer, leading to the electronic reconstructions and downshift of Mn states in the conduction band. Then, we have shown that the combination of FE polarization and antiferromagnetism can effectively tune the spin-polarized 2DEG accompanying the ferroelectric switching. In particular, imposed polarization may change the conducting state.

(3) For the $BaTiO_3/La_2CuO_4$ heterointerface based on first-principles calculations and theoretical consideration we have shown that all-oxide heterostructures incorporating ferroelectric constituent allow creating 2DEG [10]. Besides, we predicted a possibility of a high temperature guasi-two-dimensional superconductivity state in the $BaTiO_3/La_2CuO_4$ system. This state could be switchable between superconducting and conducting states by ferroelectric polarization reversal. We also discuss that such structures must be simpler for preparation. The proposed concept of ferroelectrically controlled interface superconductivity offers the possibility to design novel electronic devices.

(4) Recently, the new subject has been boosted incorporating the heterostructures based of silicon and ferroelectric perovskites, i.e., $Si/BaTiO_3$ superlattice. Recently, ferroelectrics were proposed to be used as a component for electro-optic modulators. In particular, $BaTiO_3$ is a highly promising material due to the large effective Pockels coefficient of the material, particularly in an epitaxial form. It also has the ability of being integrated on a Si material via a $SrTiO_3$ template. These two characteristics make epitaxial BTO ideal for use in next generation silicon photonics applications. We demonstrate the density of states for both heterostructure components in bulk and thin film geometries and heterointerface itself. Finally, an impact of ferroelectric polarization onto the heterostructure electronic states is analyzed also by means of ab initio computations.

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Award

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Selected Publications

1. Electronic properties of $LaAlO_3/SrTiO_3$ n-type interfaces: a GGA+U study / I.I. Piyanzina, T. Kopp, Yu.V. Lysogorskiy, D.A. Tayurskii, V. Eyert // Journal of Physics: Condensed Matter. — 2017. — V. 29, no. 9. — art. 095501.
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3. Oxygen vacancies and hydrogen doping in $LaAlO_3/SrTiO_3$ heterostructures: electronic properties and impact on surface and interface reconstruction / I.I. Piyanzina, V. Eyert, Yu.V. Lysogorskiy, D.A. Tayurskii, T. Kopp // Journal of Physics: Condensed Matter. — 2019. — V. 31, no. 29. — art. 295601.
4. Ab initio investigation of electronic and magnetic properties of antiferromagnetic/ferroelectric $LaMnO_3/BaTiO_3$ interface / V.V. Kabanov, I.I. Piyanzina, Yu.V. Lysogorskiy, D.A. Tayurskii, R.F. Mamin // Mater.Res.Express. — 2020. — V. 7, no. 5. — art. 055020.