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Analysis of electronic and structural properties of surfaces and interfaces involving $LaAlO_3$ and $SrTiO_3$ — •Irina Piyanzina[1,2], Thilo Kopp[2], and Volker Eyert[3] — [1]Institute of Physics, Kazan Federal University, Kremlyovskaya St. 18, 420008 Kazan, Russia — [2]EP VI and Center for Electronic Correlations and Magnetism, Universität Augsburg, Universitätsstraße 1, D-86135 Augsburg, Germany — [3]Materials Design SARL, 18 rue de Saisset, 92120 Montrouge, France

Recently, it was established that a two-dimensional electron system can arise at the interface between the two oxide insulators $LaAlO_3$ (LAO) and $SrTiO_3$ (STO) [A. Ohtomo and H. Hwang, Nature **427**, 423 (2004)., S. Thiel et al., Science **313**, 1942 (2006)]. This paradigmatic example furthermore exhibits magnetism between the non-magnetic oxides. Despite the huge amount of both theoretical and experimental work a thorough understanding has yet to be achieved.

The aim of the present study is to investigate the electronic properties and structural distortions of surfaces and interfaces based on LAO and STO by means of density functional theory. We analyzed the structural deformations of the $LaAlO_3$ (001) slab induced by hydrogen adatoms and oxygen vacancies at its surface. Moreover, we investigated the influence of surface reconstruction on the density of states and determined the spatial dependence of the density of state at the Fermi level for bare $LaAlO_3$ surfaces and $LaAlO_3/SrTiO_3$ interfaces. In addition, the Al-atom displacements and distortions of the TiO_6-octahedra were estimated.

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