J. At. Mol. Sci.
doi: 10.4208/jams.091012.100312a

Vol. **4** , No. 3 , pp. 280-286
August 2013

First-principles study of electronic structure and optical properties of the $LaAlO_3/SrTiO_3$ interfaces

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Received 10 September 2012; Accepted (in revised version) 3 October 2012
Published Online 28 June 2013

Abstract. The electronic structure and optical properties of the perovskite oxide $LaAlO_3$, $SrTiO_3$ and $LaAlO_3$ /$SrTiO_3$ interfaces were studied by the density functional theory (DFT) based on First-principles plane wave pseudopotential method. The energy band structure analysis shows that the $(AlO_2)^-/(TiO_2)^0$ interface is insulating with the band gap being 1.888 eV, whereas the $(LaO)^+/(SrO)^0$ interface seems to be a semiconductor or semimetal with the band gap being 0.021 eV. Moreover, we have also investigated optical properties of the $LaAlO_3$, $SrTiO_3$ and $LaAlO_3/SrTiO_3$ interfaces, the results indicate that the intensities of absorption, reflectivity, and energy loss spectra of $LaAlO_3$ and $SrTiO_3$ are higher than the corresponding intensities of the $LaAlO_3$ /$SrTiO_3$ interfaces.

PACS: O562.1

Key words: $LaAlO_3/SrTiO_3$ interface, electronic structure, optical properties, first principles

1 Introduction

In recent years, the heterointerfaces of the perovskite oxide have been greatly studied because of their huge application for electronic devices, such as field-effect transistors, bipolar transistors, and light emitting diodes [1], and because of these perovskite oxides have simple atomic structures and rich physical properties, which can realize the change of magnetic - nonmagnetic, metallic - insulated by means of atomic change [2].

Ohtomo *et al.* [3] fabricated the atomic-scale $LaTiO_3$ (LTO)/$SrTiO_3$ (STO) heterointerfaces and observed the spatial distribution of the extra electron on the titanium sites even

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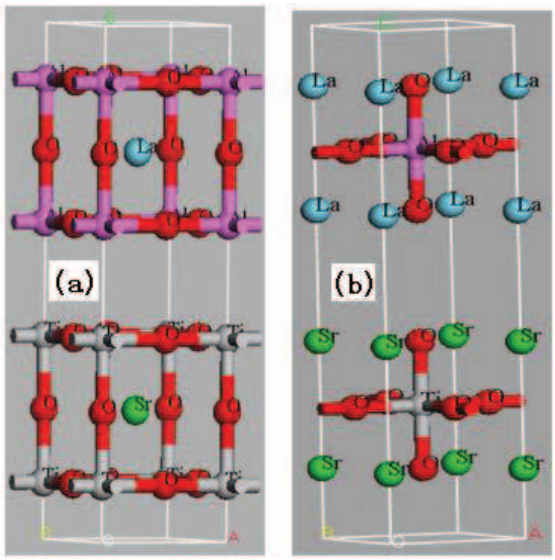

Figure 1: The interface structure configurations of LAO/STO (a) $(AlO_2)^-/(TiO_2)^0$ interface; (b)$(LaO)^+/(SrO)^0$ interface.

though the superlattice structure is based on two insulators, and suggested that the extra electron could be driven by the presence of charged donor LaO layers. Later, Ohtomo and Hwang [4] found a high mobility electron gas at $LaAlO_3$(LAO)/STO heterointerface and considered that the properties of interface is depend on the structure of the interface. The hole-doped interface $(AlO_2)^-$ / $(SrO)^0$ (AO-SO) is found to be insulating, whereas the electron-doped interface $(LaO)^+$ / $(TiO_2)^0$(LO-TO) is conducting. Nakagawa *et al.* [5] proposed a simple electrostatic model. Thiel *et al.* [6] suggested that the conductivity of the electron gases can be modulated through a quantum phase transition from an insulating to a metallic state. Meanwhile, various theoretical and experimental studies have attracted attention [7-16]. Until now, the electrical and optical properties of $(AlO_2)^-$/ $(TiO_2)^0$ (AO-TO) and $(LaO)^+$/ $(SrO)^0$ (LO-SO) interfaces have been little known. Therefore, investigation into the electronic and optical properties of LAO/STO interfaces is relevant and intriguing.

2 Models and methods

The present calculations were performed with CASTEP code based on density functional theory [17]. All possible structures are optimized by the BFGS algorithm, which provides a fast way of finding the lowest energy structure. Further, the optimization is performed until the forces on the atoms diminish to less than 0.05 eV/Å, and on all the stress components, to less than 0.1 GPa. The tolerance in the self-consistent field (SCF) calculation is 2.0×10^{-5} eV/atom. Ultrasoft pseudopotentials are expanded within a plane-wave basis