Origin of Two-dimensional Electron Gas at (110) $LaAlO_3/SrTiO_3$ Interface: First-principle Study and XPS Investigation

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Introduction

The observation of a high-mobility two-dimensional electron gas between two insulating complex oxides, especially (001) $LaAlO_3/SrTiO_3$[1-3], has enhanced the potential of oxides for electronics. The conductivity in crystalline (001) $LaAlO_3/SrTiO_3$ interface is mostly interpreted to originate from electronic reconstruction,which is a direct consequence of the polarization discontinuity[1]. For (001)-oriented LAO/STO interfaces, it exhibits polar discontinuity because of the alternate stacking of $[LaO]^+[AlO_2]^-$ planes over $[SrO]^0[TiO2]^0$ (**Figure 1a**), while for (110)-oriented LAO/STO interfaces (**Figure 1b**), it doesn't exihibit any polar discontinuity acacording to the stack sequence $[ABO]^{4+}/[O2]^{4-}$ along [110] orientation. Thus (110) LAO/STO interface has been generally accepted to be a insulating interface whithout displaying any electronic reconstruction. In the present work, we investigate the electronic structure and band alignment of (100) LAO/STO interface combining density-functional calculation with X-ray photoelectron spectroscopy.

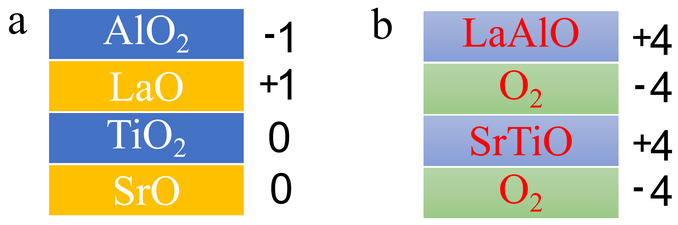
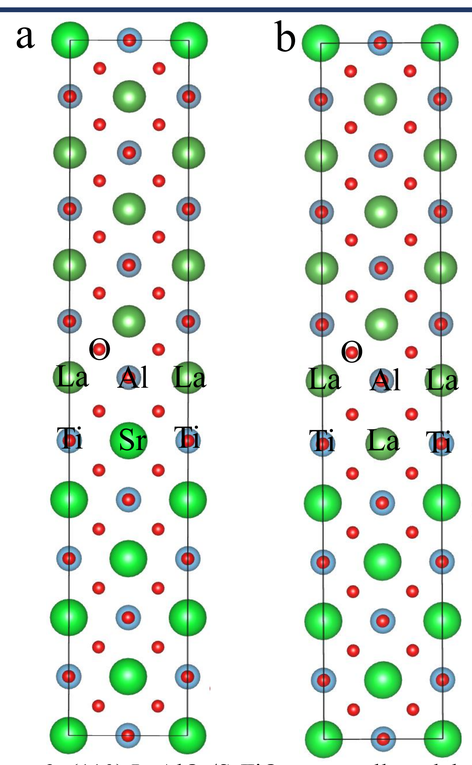


Figure 1. Layout of the polar catastrophe model for $LaAlO_3/SrTiO_3$ interface on (a) (001)- and (b) (110)- orientations, where planes are segmented as planar charge sheets..

Models and samples



Models in theory

A perfect structure (**Figure 2a**)and a cation diffusion structure (**Figure 2b**) were constructed **in our calculation**.

Samples preparation

In the experiment, $LaAlO_3$ films was grown in a step-flow mode on (110) $SrTiO_3$ substrate and well epitaxial $LaAlO_3$ films were gained.

Figure 2. (110) $LaAlO_3/SrTiO_3$ supercell models. (a) is a perfect structure which joints ideal $LaAlO_3$ and $SrTiO_3$ on 110- orientation; (b) is a cation diffusion model, in this case, Ti atoms are substituted by La atoms at the interface to simulate cation diffusion.

Methods

Calculation part

Projected augmented wave method with a plane wave basis set as implemented in the Vienna ab initio Simulation Package (VASP) is used. The exchange-correlation potential is treated in local density approximation (LDA)

Experiment part

The XPS data were obtained using an ESCA Lab250 electron spectrometer with monochromatic 150 W Al Kα radiation as the x-ray source.The obtained XPS data were processed using *Thermo Avantage* software.

References

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Results and discussions

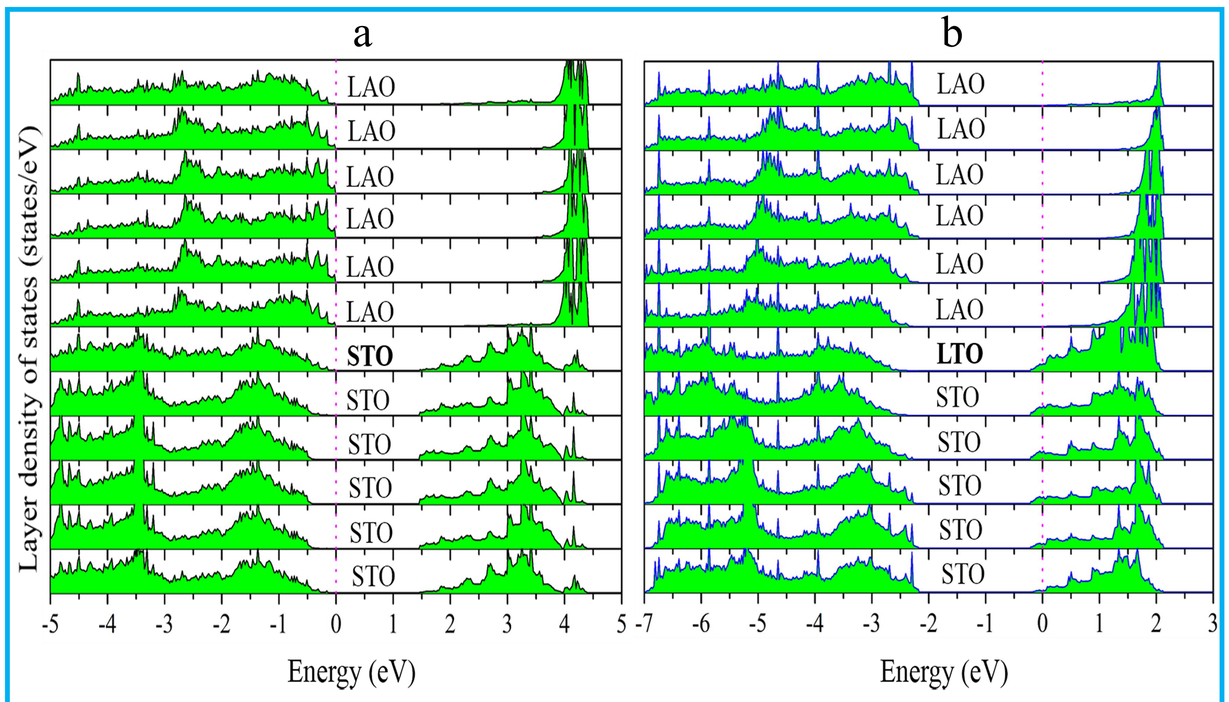

Figure 3. Layer density of states of (a) perfect (110) LAO/STO supercell and (b) La diffusion (110) LAO/STO supercell. Insulator-to-Metal transition is induced by cation diffusion.

The calculated layer density of state of perfect (110) LAO/STO supercell and cation diffusion (110) LAO/STO supercell are presented in Figure 3. In the case of perfect supercell (**Figure 3a**), an obvious band gap of 1.5 eV is shown and the valance band of $SrTiO_3$ is flat, thus exhibiting a insulator interface. On the contrary, within the scenario assuming La diffusion (**Figure 3b**), electrons spread into Ti-3d orbitals and force the Fermi level to shift into conduction band, resulting in two-dimensional electron gas at the interface. Especially, the bands bending at the both sides of $LaAlO_3$ and $SrTiO_3$ is corresponding to band alignment of (110) LAO/STO interface (**Figure 4**) acquired in our XPS measurement.

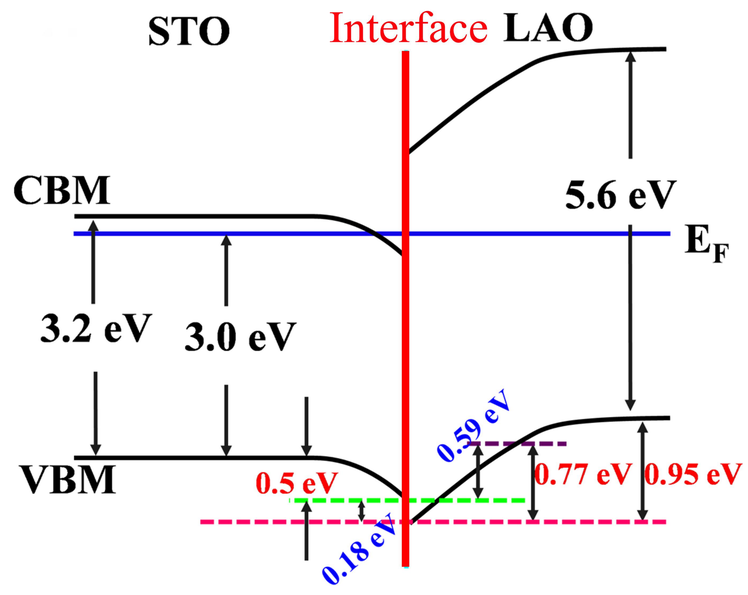

Figure 4. The detailed band alignment of (110) LAO/STO interface. It is clearly observed that a notched structure cut by Fermi level locates inside the $SrTiO_3$ side.

Conclusion

- The layer density of states in DFT calculation shows cation diffusion-induced two dimensional electron gas at (110) LAO/STO interface.
- The band bending in layer density of states is in agreement with that from band alignment diagram, which proves that La diffuses into $SrTiO_3$ forming $La_{1-x}Sr_xTiO_3$ layer.
- We suggest a interface doping meachnism to explain the origin of two dimensional electron gas at (110) LAO/STO interface.

Acknowledgments

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