

## Controlling band alignments by engineering interface dipoles at oxide heterointerfaces

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### Introduction

Band offsets, which define the properties of various electronic devices, are in principle uniquely determined by parameters such as the work function and the electron affinity. In practice, the formation of an interface dipole (electric double layer) can modify the band offset, opening up the possibility of great enhancement in device functionality. This dipole engineering, however, is often problematic. For example, attempts to engineer dipoles at conventional metal/semiconductor interfaces, which form Schottky junctions, are hindered by the presence of interface states. Ionic materials, on the other hand, are sometimes free from this obstacle [1], facilitating the formation of dipoles simply by the accurate positioning of the required charges, one after another. Here, in oxides with strong ionic character, we succeeded in creating a huge electric dipole by sequentially fabricating ionic layers on the atomic scale at a metal/semiconductor interface. By varying the type and number of embedded ions, the sign and magnitude of the interface dipole was tuned giving up to the total range of 1.7 eV variation in the Schottky barrier height (SBH), facilitating the design of an arbitrary SBH independently of the metal work function or the semiconductor electron affinity.

### Results and Discussions

The (001)-oriented SrRuO<sub>3</sub>/Nb:SrTiO<sub>3</sub> interface, which consists of materials with a common perovskite crystal structure ABO<sub>3</sub>, was chosen as the model system for dipole engineering. In this ABO<sub>3</sub> framework a “charged layer” of either (LaO)<sup>+</sup> or (AlO<sub>2</sub>)<sup>-</sup> was inserted, to form a dipole with the counter (screening) charge in the metallic SrRuO<sub>3</sub> [Figs. 1a and b]. Current-voltage characteristics, capacitance-voltage characteristics, internal photoemission spectra, and X-ray photoemission spectra (PES) [Fig. 2] showed that the Schottky barrier height was tuned in a broad range from 0 eV (Ohmic contact) to 1.7 eV, with respect to the original value of 1.2 eV. These results demonstrate arbitrary control of the band offsets at oxide heterointerfaces, implying a large degree of freedom to use oxides for structures in conventional as well as strongly correlated devices.

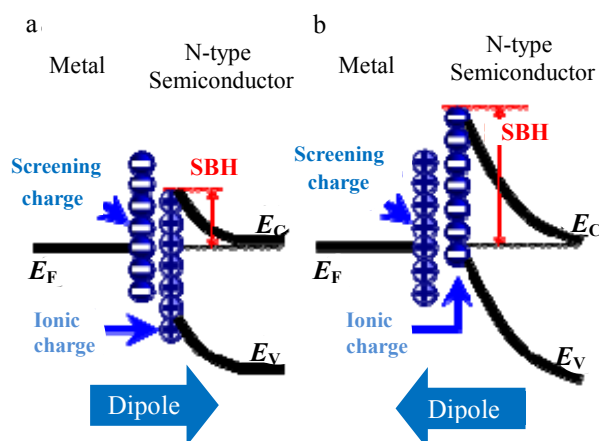


Fig. 1 Schematics of interface dipoles created between inserted ionic charges and induced screening charges. SBH is **a** increased and **b** decreased by interface dipoles.

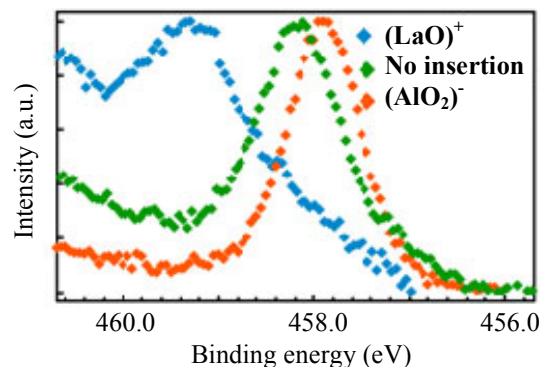


Fig. 2 PES spectra for Ti  $2p_{3/2}$  core levels in SrRuO<sub>3</sub>/Nb:SrTiO<sub>3</sub> Schottky junctions, whose interfaces were engineered in three different ways: (LaO)<sup>+</sup> insertion, no insertion, and (AlO<sub>2</sub>)<sup>-</sup> insertion.

### References

[1] S. Kurtin, T. C. McGill, and C. A. Mead, Phys. Rev. Lett. **22**, 1433 (1969).

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