Supplementary Information

First-principles studies of ensional electron gas at the interface of polar/pol $_3$/$KNbO_3$ superlattices

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Superlattice model (without vacuum) and slab model (with vacuum) both are computationally feasible to explore whether there exists a critical thickness. The details about that are available in the References: Adv. Mater. 2010, 22, 2881 and Phys. Rev. B 2009, 80, 045425. We think there would be surface effects in the slab model (with vacuum), which can affect the accuracy of interface properties. Therefore, in the main text we chose the superlattice model (without vacuum) with periodic boundary conditions, which should be more reasonable to mimic experimental situation where epitaxial perovskites can be grown layer by layer on the substrate. Here we have also constructed and calculated the freestanding $LaAlO_3$/$KNbO_3$ (LAO/KNO) heterostructures with vacuum by using the same parameters in the text. By comparison of Figure S1 here and Figure 2 in the main manuscript, we found that the slab model with vacuum is more likely to produce metallic states, and the results confirmed the conclusion in the paper (Adv. Mater. 2010, 22, 2881-2899).

We also considered carefully the difference of the polarized atomic layer and intrinsic ferroelectric polarization in $KNbO_3$. In detail, we calculate electronic band structures of the unrelaxed $(LaAlO_3)_{4.5}$/$(KNbO_3)_{8.5}$ and $(LaAlO_3)_5$/$(KNbO_3)_8$ superlattices without intrinsic ferroelectric polarization of $KNbO_3$ due to atomic displacements. We can learn from Figure S2 that the charge-polarized atomic layer and the ferroelectric polarization take opposite effects, i.e. the presence of ferroelectricity weakens the concentration of 2DEG or 2DHG.

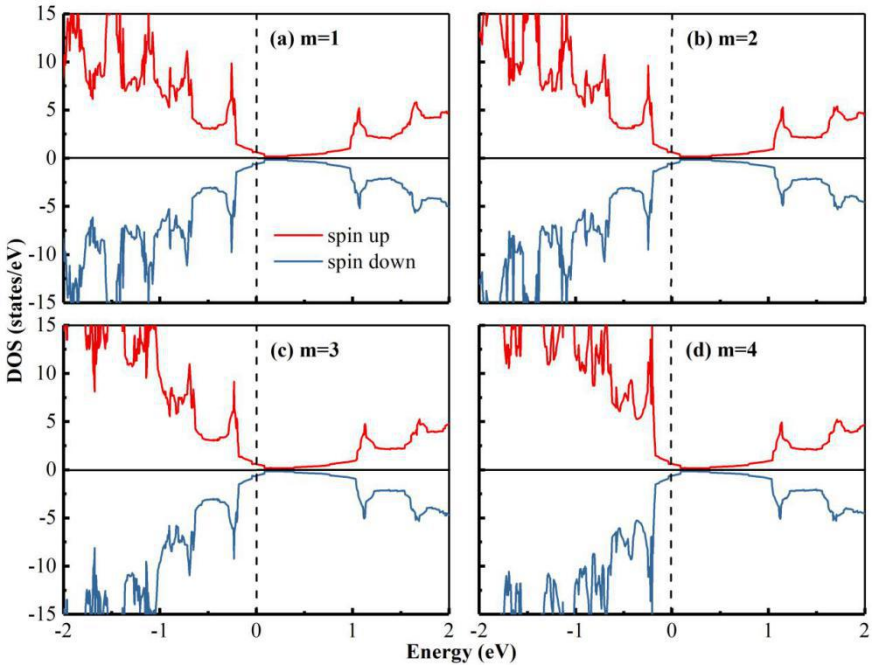

Figure S1 The calculated spin-resolved total density of states (DOS) for the stoichiometric $(LaAlO_3)_m/(KNbO_3)_8$ *slab* systems with vacuum (m=1, 2, 3, 4).

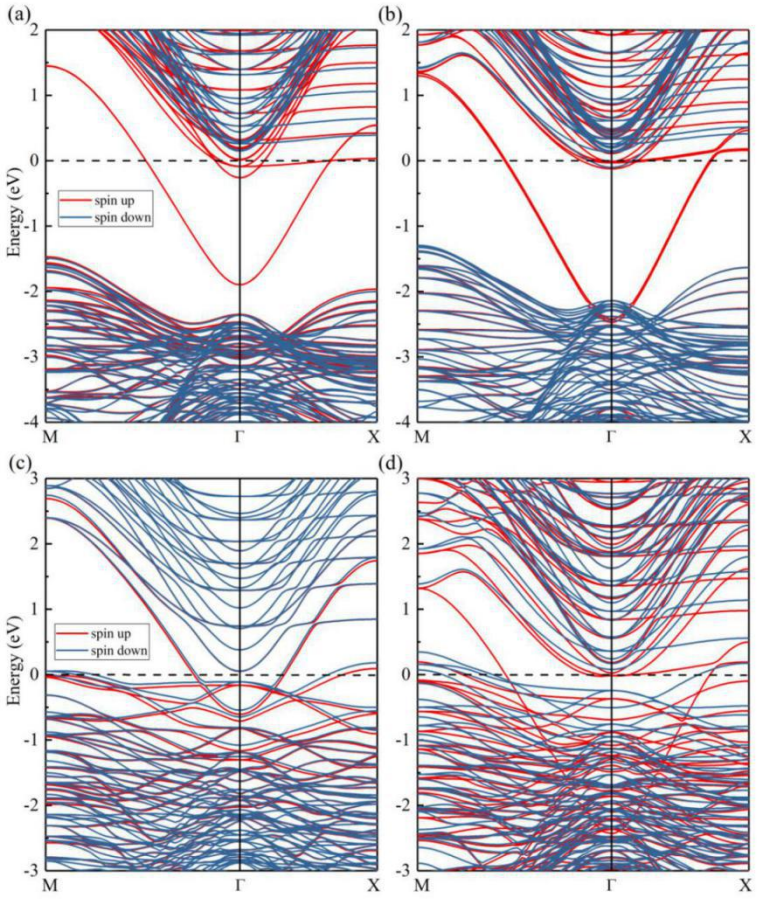

Figure S2 Calculated electronic band structures for (a) the relaxed ferroelectric KNO and (b) unrelaxed paraelectric KNO $(LaAlO_3)_{4.5}/(KNbO_3)_{8.5}$, respectively. (c) and (d) are electronic band structures of relaxed and unrelaxed $(LaAlO_3)_5/(KNbO_3)_8$ superlattices respectively.