

Supplementary Information

The two-dimensional n/p type carriers at the interface of $\text{LaAlO}_3/\text{KTaO}_3$ heterostructures

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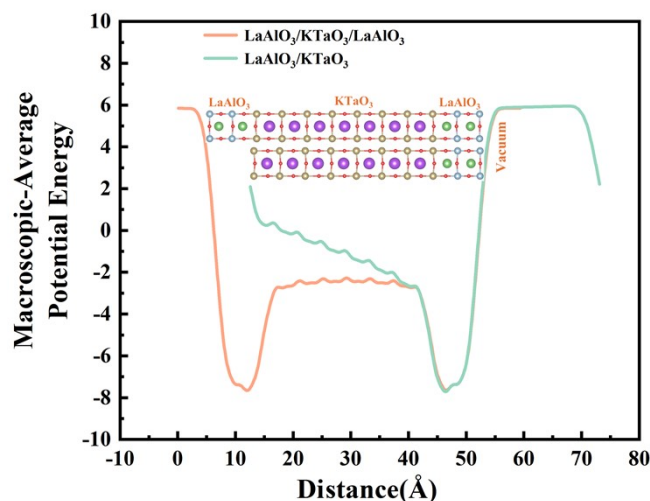


FIG. S1 The macroscopically averaged potentials are plotted along the [001] direction of the n -type interface $(\text{LaAlO}_3)_2/(\text{KTaO}_3)_8$ and $(\text{LaAlO}_3)_2/(\text{KTaO}_3)_{7.5}/(\text{LaAlO}_3)_2$ heterostructure.

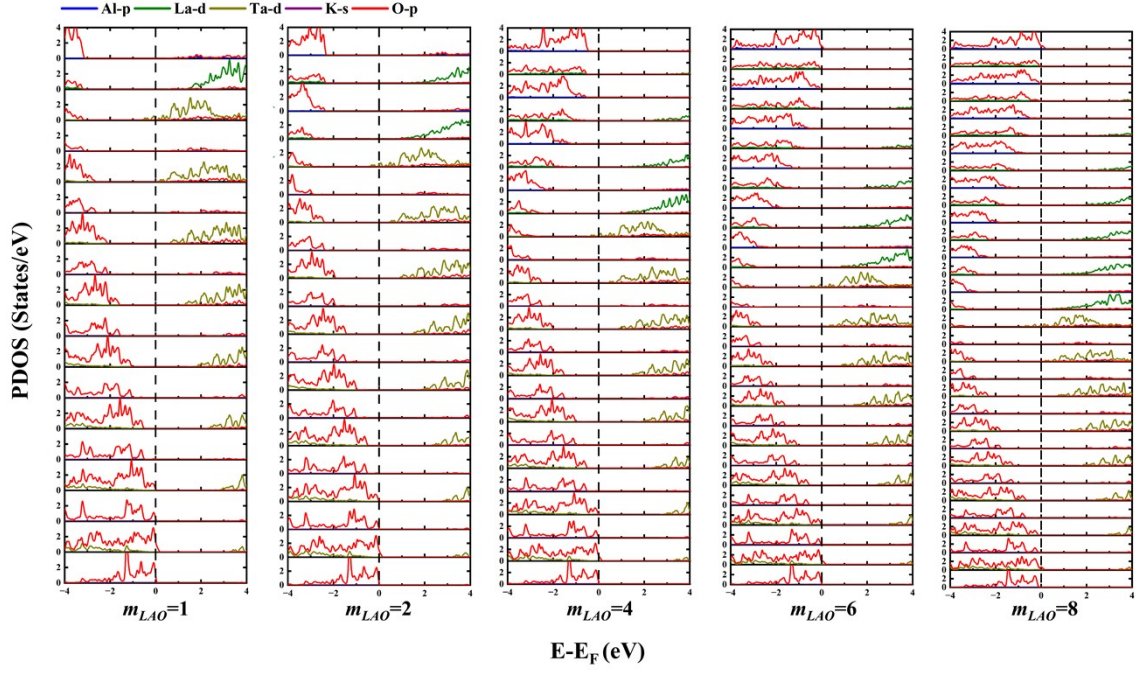


FIG. S2 Calculated layer-resolved PDOS for the n -type $\text{LaO}^+/\text{TaO}_2^+$ interfaces of $(\text{LaAlO}_3)_m/(\text{KTaO}_3)_8$ heterostructure slab models with $m=1, 2, 4, 6, 8$.

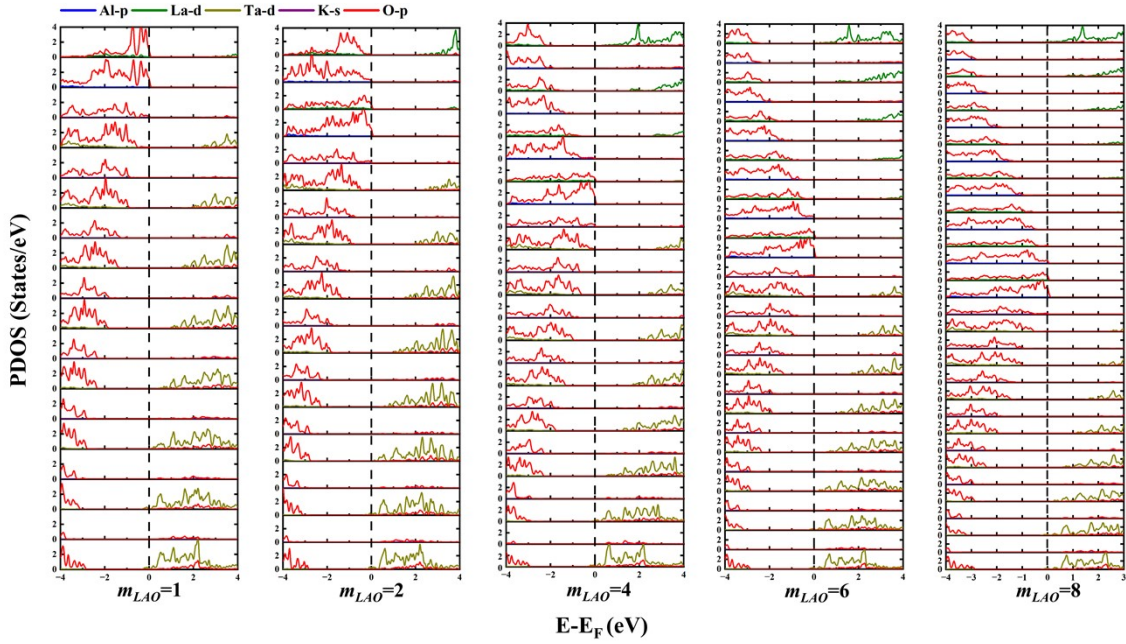


FIG. S3 Calculated layer-resolved PDOS for the p -type $\text{AlO}_2^-/\text{KO}^-$ interfaces of $(\text{LaAlO}_3)_m/(\text{KTaO}_3)_8$ heterostructure slab models with $m=1, 2, 4, 6, 8$.

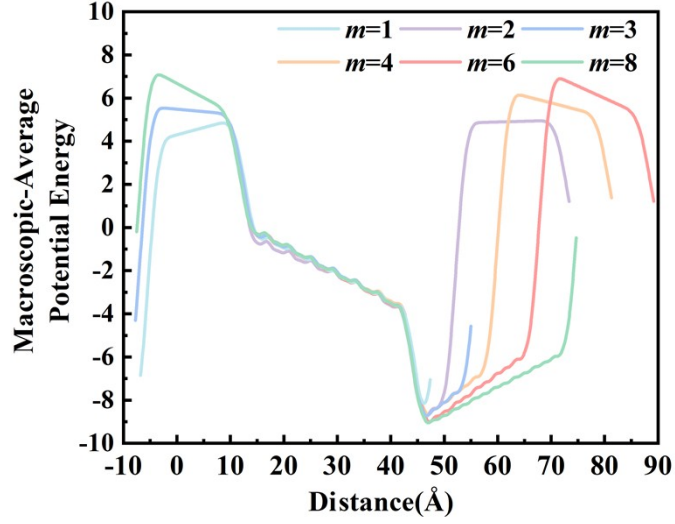


FIG. S4 The macroscopically averaged potentials are plotted along the $[001]$ direction of the n -type $(\text{LaAlO}_3)_m/(\text{KTaO}_3)_8$ heterostructure slab models with $m=1, 2, 3, 4, 6, 8$.

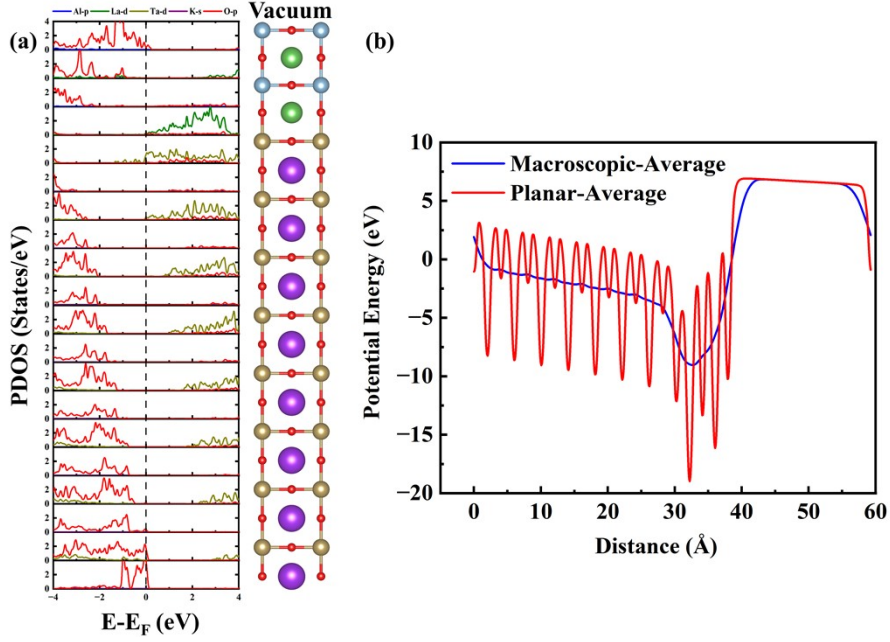


FIG. S5 (a) Calculated layer-resolved PDOS for n -type $\text{LaO}^+/\text{TaO}_2^+$ interfaces of $(\text{LaAlO}_3)_2/(\text{KTaO}_3)_8$ heterostructure slab models without structure relaxation. (b) The local electrostatic potential (red line) and macroscopically averaged potential (blue line) are plotted along the $[001]$ direction of the heterostructure.

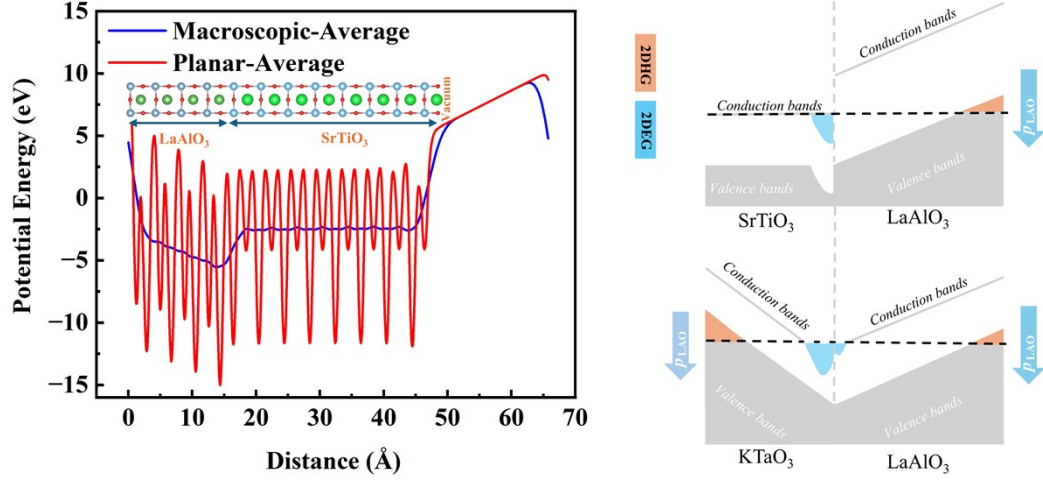


FIG. S6 The local electrostatic potential (red line) and macroscopically averaged potential (blue line) are plotted along the $[001]$ direction of the n -type $(\text{LaAlO}_3)_4/(\text{SrTiO}_3)_8$ heterostructure with perfect structure relaxation. The heterostructure model is shown as inset; The schematic diagrams of band alignment in different structural models (right), where p stands for the initial polarization of LaAlO_3 or KTaO_3 .

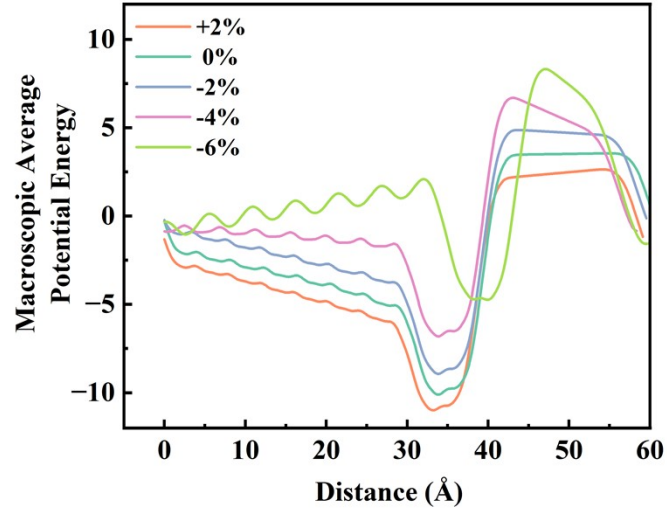


FIG. S7 The macroscopically averaged potentials are plotted along the $[001]$ direction of the n -type $(\text{LaAlO}_3)_2/(\text{KTaO}_3)_8$ heterostructure with in-plane strain of 2%, 0%, -2%, -4%, -6%.

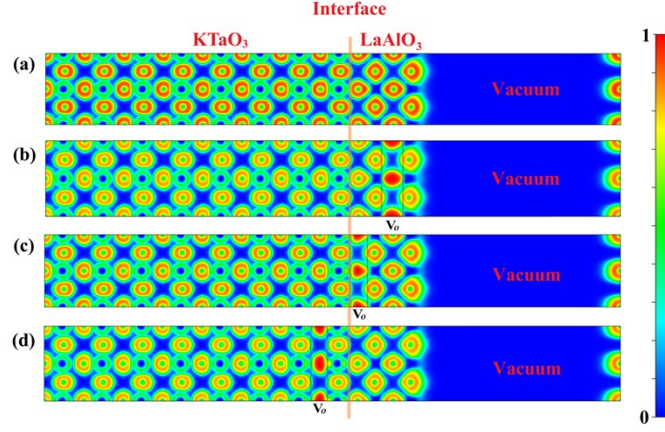


FIG. S8 The electron localization function (ELF) is plotted along the [001] direction of the n -type interface $(\text{LaAlO}_3)_2/(\text{KTaO}_3)_8$ heterostructure with pure (a) and O vacancy defect (b-d) located at layer 2, 4, 6.

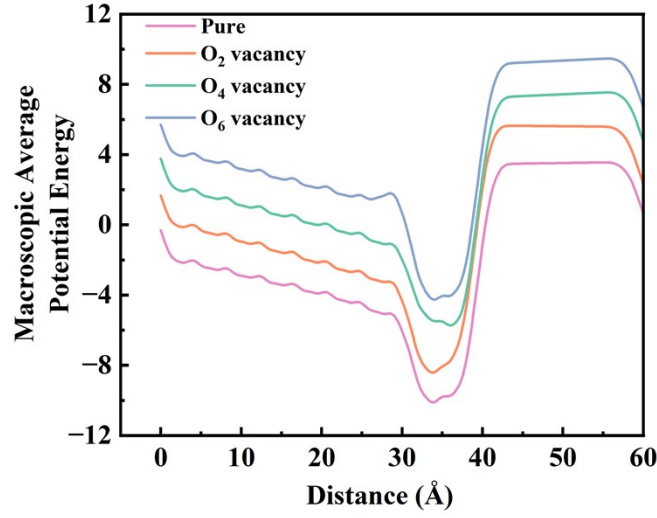


FIG. S9 The macroscopically averaged potentials are plotted along the [001] direction of the n -type interface $(\text{LaAlO}_3)_2/(\text{KTaO}_3)_8$ heterostructure with O vacancy defect located at layer 2, 4, 6.