Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Strain-driven carrier-type switching of surface two-dimensional electron and hole gases in $KTaO_3$ thin film

Xue-Jing Zhang[1,2] and Bang-Gui Liu[1,2,*]

[1] *Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China*

[2] *School of Physical Sciences, University of Chinese Academy of Sciences, Beijing 100190, China*

In Fig. S1, we present the band structures of the $(KTO)_{12}$ slab with the correlation parameter $U = 3$ eV, for different strain values: ε_s=0%, 5%, -1%, -2%, -3%, -4%, -5%, and -6%.

In Fig. S2 presented are the monolayer-resolved z-axis displacements of cations with respect to the nearest O anions of the $(KTO)_{12}$ slab at different in-plane strain values: 0%, ±1%, ±2%, ±3%, ±4%, and ±5%. The displacement is a sum of those originating from Ta and K atoms in the monolayer of the unit-cell thickness. The contribution of K is multiplied by 5 to get regular curves. The values at the surfaces are made by comparing with the ideal atomic positions.

In Fig. S3, we present the band structures of the $(STO)_{12}$ slab at different strain values: ε_s=0%, 5%, -1%, -2%, -3%, -4%, and -5%.

In Fig. S4, we present the band structures of the $(KTO)_6$ slab at different in-plane strain values: 0%, ±1%, ±2%, ±3%, ±4%, and ±5%. The spectral weights of Ta atoms at the top and bottom surfaces are emphasized.

In Fig. S5, we present the electronic band structures of the bulk KTO, bulk LAO, and bulk STO, calculated with PBEsol.

In Fig. S6, we present the band structures of $(KTO)_{12}/(LAO)_6$ and $(KTO)_{12}/(STO)_6$ with the other interfaces.

* bgliu@iphy.ac.cn

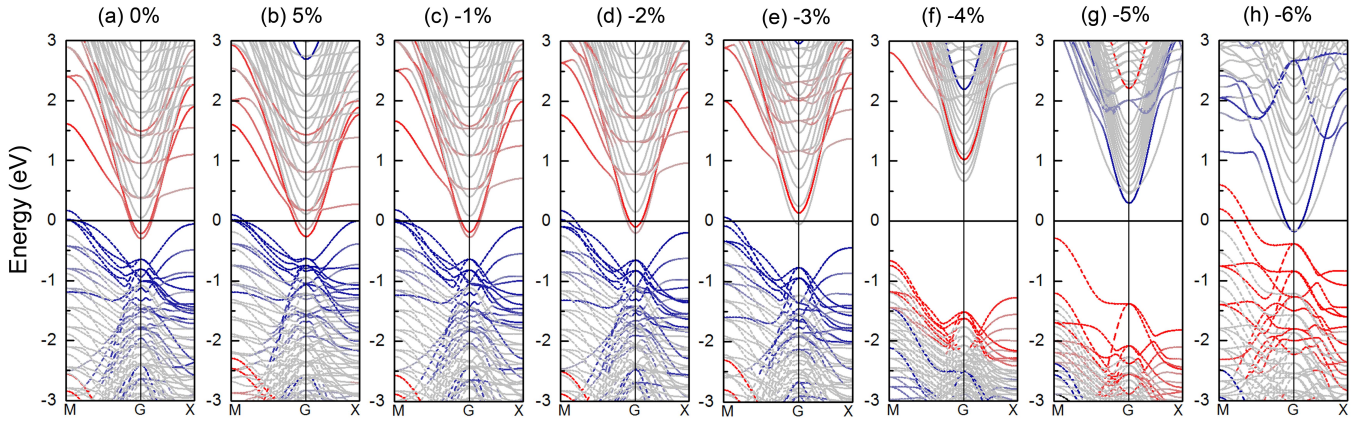

FIG. S1. (Color online) Band structures of the $(KTO)_{12}$ slab with $U = 3$ eV at different strain values: ε_s=0%, 5%, -1%, -2%, -3%, -4%, -5%, and -6%. The red and blue lines in the conduction bands describe the energy bands originating from Ta atoms of the monolayers labelled with 'XII' and 'I', respectively. The red and blue lines in the valence bands indicate the energy bands originating from O atoms in the top and bottom surfaces, respectively.

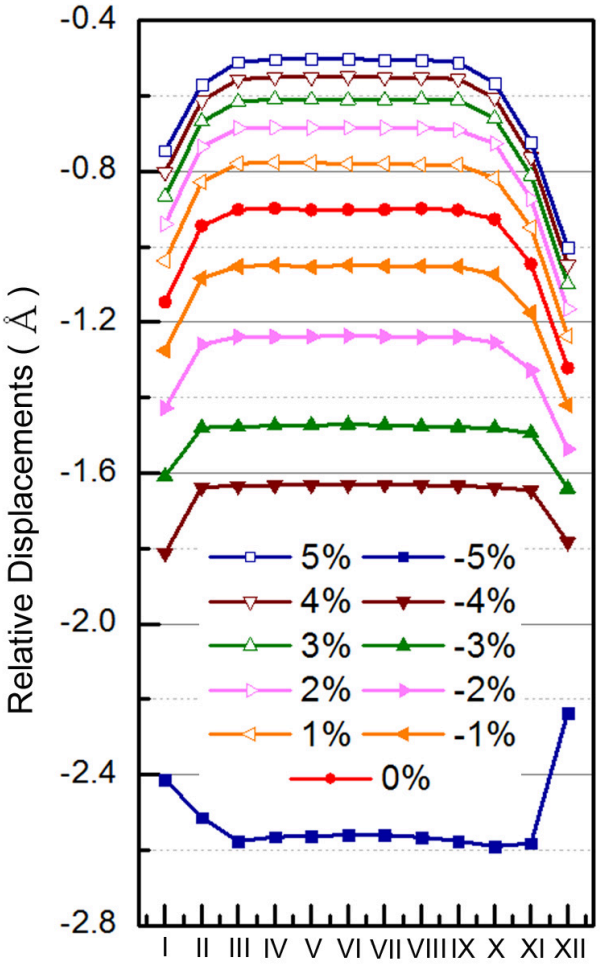

FIG. S2. (Color online) The monolayer-resolved displacements along the z axis of cations with respect to the nearest O anions of the KTO slab for different strain values: 0%, ±1%, ±2%, ±3%, ±4%, and ±5%.

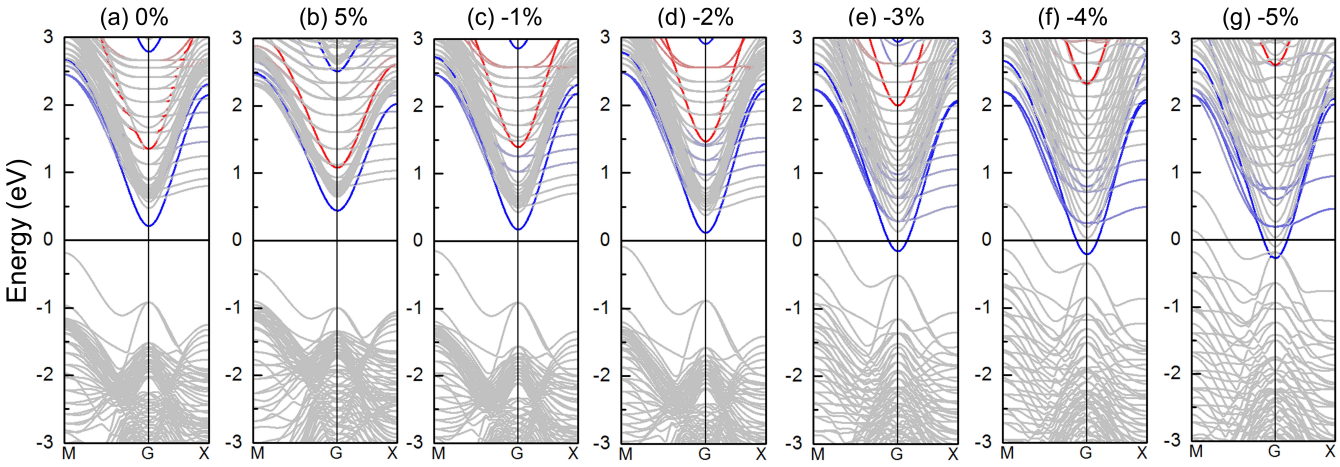

FIG. S3. (Color online) Band structures of the $(STO)_{12}$ slab at different strain values: ε_s=0%, 5%, -1%, -2%, -3%, -4%, and -5%. The red and blue lines in the conduction bands describe the energy bands originating from Ti atoms of the monolayers labelled with 'XII' and 'I', respectively.

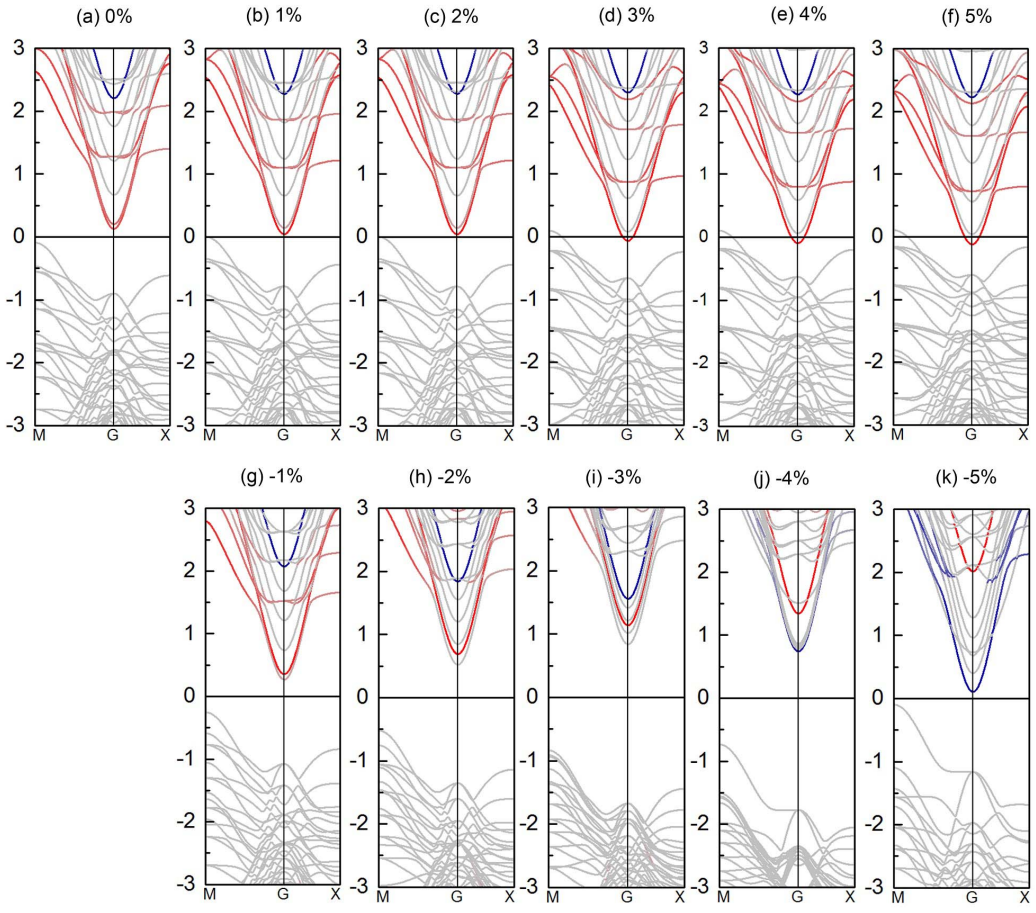

FIG. S4. (Color online) Band structures of the KTO slab with $m = 6$ at ε_s=0%, 1%, 2%, 3%, 4%, 5%, -1%, -2%, -3%, -4%, and -5%. The red and blue lines indicate the bands originated from Ta atoms in the TaO_2 monolayer at the top and bottom surfaces, respectively.

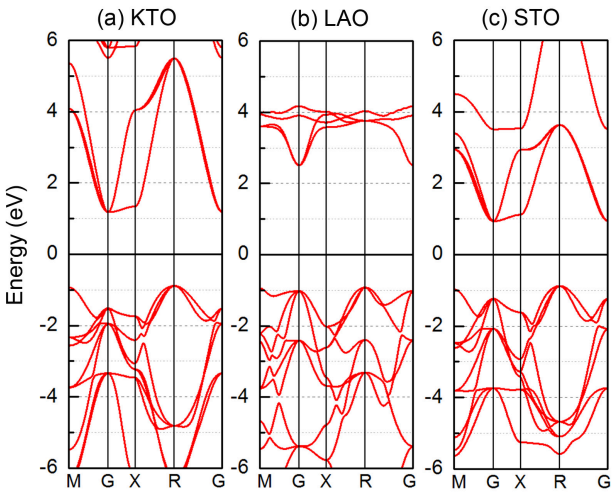

FIG. S5. (Color online) Electronic band structures of the bulk KTO (a), bulk LAO (b), and bulk STO (c) calculated with PBEsol.

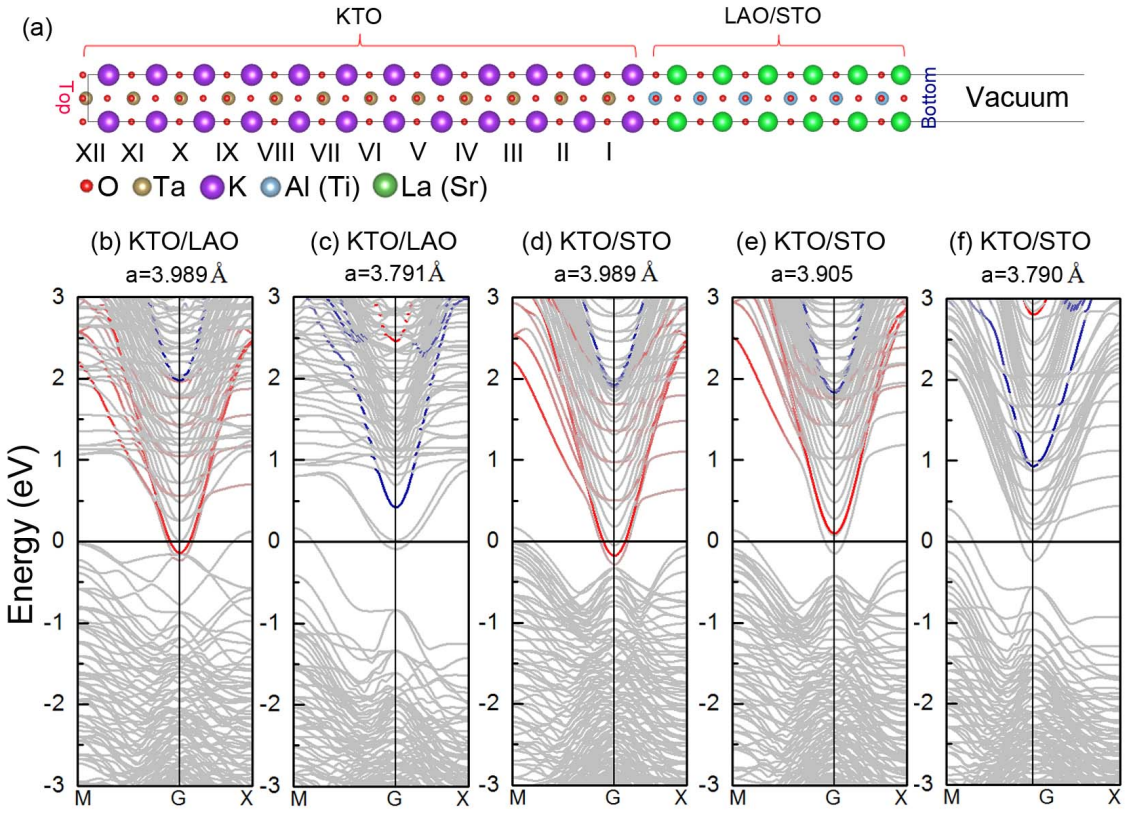

FIG. S6. (Color online) (a) Side view of crystal structure of $(KTO)_{12}/(LAO)_6$ or $(KTO)_{12}/(STO)_6$ with the other interfaces. (b)-(c) The band structures of $(KTO)_{12}/(LAO)_6$ for $a_{\parallel} = a_{KTO}$ (b) and $a_{\parallel} = a_{LAO}$ (c). (d)-(f) The band structures of $(KTO)_{12}/(STO)_6$ for $a_{\parallel} = a_{KTO}$ (d), $a_{\parallel} = a_{STO}$ (e), and $a_{\parallel} = 3.790$ Å (f). The red and blue lines in the conduction bands describe the energy bands originating from Ta atoms of the monolayers labelled with 'XII' and 'I', respectively.