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Interface enhanced functionalities in $BaTiO_3/CaTiO_3$ superlattices

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Interface engineering of oxide thin films has led to the development of many intriguing physical properties and new functionalities, in which the oxygen rotation and tilting take an crucial role. The oxygen octahedral tilt has been considered to be a coherent motion in the oxide thin-films, based on which the tilt is often neglected in the modeling of ABO_3 superlattices. However, combined with state-of-art experimental high-resolution electron microscopic image, our first-principles results clearly show that oxygen octahedral tilt should be more appropriately defined by the tilting angles of two individual pyramids. Each pyramid will tilt rather independently as a function of its local chemical environment. Considering the oxygen octahedral rotation at the same time, the new picture of oxygen octahedral tilting will induce a novel interface effect, in which an unstable structure in bulk $CaTiO_3$ will be stabilized at the interface in $BaTiO_3/CaTiO_3$ superlattice. This novel interface effect induces large polarizations both in-plane and out-of-plane with a corresponding enhanced piezoelectricity. The above scenario successfully explains the recent experimental discoveries in $BaTiO_3/CaTiO_3$ superlattices by H. Lee's and P. Evan's groups respectively.