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Oxygen vacancy shuttle across the LaAlO3/SrTiO3 interface EVGENY Y. TSYMBAL, TULA R. PAUDEL, YONG WANG, J.D. BURTON, University of Nebraska, Lincoln — There have been several recent indications of a switchable piezo-response in oxide materials not associated with ferroelectric polarization. We explore a LaAlO3/SrTiO3 (LAO/STO) heterostructure as a model system to understand this behavior by considering oxygen vacancies as the origin. Using first-principles calculations based on a supercell approach and an adequate electrostatic model, we show that the oxygen vacancy formation energy has two local minima: one at the surface of LAO and another in STO few unit cell below the interface. Due to inbuilt electric field in the system, electrons forming the oxygen vacancies in LAO transfer to the interface leaving behind two holes at the vacancy site irrespective of their spatial position, whereas those in the STO exhibit such a behavior only when laying within a finite distance ∼1nm associated with the screening length of the electric field in STO. The two local minima may accommodate oxygen vacancies reversibly when the applied electric field changes its polarity producing a switchable piezo-response behavior in the LAO/STO system.

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