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Oxygen-vacancy-induced charge carrier in n-type interface of $LaAlO_3$ overlayer on $SrTiO_3$ (001): interface vs bulk doping carrier YUN LI, SUTASSANA NA PHATTALUNG, JAEJUN YU, Department of Physics and Astronomy, FPRD, Center for Strongly Correlated Materials Research, Seoul National University, Seoul 151-747 — We investigated the role of oxygen vacancy at the n-type interface of $LaAlO_3$ (LAO) overlayer on $SrTiO_3$ (STO) (001) by carrying out density-functional-theory calculations. We found that regardless of the concentration of oxygen vacancies there are always oxygen vacancies formed in LAO surface. The oxygen vacancies in the surface induce a two-dimensional carriers of no more than 0.5 electron per two-dimensional unit cell at the interface, which partially or completely compensate the polar electric field in LAO and lead to band bending at the interface in STO side. In addition, oxygen vacancies may be formed uniformly in STO for the configuration with high concentration of vacancies. Our calculations show that every oxygen vacancy in STO donates two electron carriers. We ascribed the three-dimensional distribution of higher density of carriers found in experiments to the large amount of vacancies in STO.

Yun Li

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