Electronic structure of interfaces between insulating LaAlO$_3$ and SrTiO$_3$ perovskite oxides

MIN SIK PARK, S.H. RHIM, A.J. FREEMAN, Northwestern University — Since heteroepitaxial structures of perovskite oxides are potent candidates for multifunctional devices, understanding their interface properties is very important for applications, because they often show completely different properties from bulk. Recently, interfaces between the wide-band gap insulators of LaAlO$_3$ and SrTiO$_3$, were found to be insulating when hole-doped, and conducting when electron-doped. First-principles calculations with the highly precise full-potential linearized augmented plane wave (FLAPW) method for the stoichiometric compounds on [001] superlattices composed of perovskite unit cells of LaAlO$_3$ and SrTiO$_3$, show metallicity in both the hole-doped AlO$_2$/SrO and electron-doped LaO/TiO$_2$ interfaces, even with inclusion of geometry relaxation. Only by considering oxygen vacancies is the experimental result of insulating behavior in the hole-doped AlO$_2$/SrO interface obtained.

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