Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Electronic structure of interfaces between insulating $LaAlO_3$ and $SrTiO_3$ perovskite oxides[1] 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 [2]. First-principles calculations with the highly precise full-potential linearized augmented plane wave (FLAPW) method [3] 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.

[1]Supported by KRF Grant (KRF-2005-214-C00035) and NSF through the NU MRS Grant (DMR-0076097)
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Date submitted: 19 Dec 2005 Electronic form version 1.4