Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Density-functional Study of Suppressed Magnetism at $La_{0.7}Sr_{0.3}MnO_3/SrTiO_3$ Interfaces[1] JUN HE, Vanderbilt University, ALBINA BORISEVICH, SERGEI KALININ, STEPHEN PENNYCOOK, Oak Ridge National Laboratory, SOKRATES PANTELIDES, Vanderbilt University — The experimentally observed magnetism suppression at interfaces of $La_{0.7}Sr_{0.3}MnO_3$ has attracted increasing attention. Here we report density-functional calculations for the interface systems of $La_{0.7}Sr_{0.3}MnO_3/SrTiO_3$. Two interface models are employed to isolate and identify different effects coming from epitaxial strain, symmetry-breaking, charge redistribution, and oxygen vacancy segregation. We found that the strain effect from $SrTiO_3$ substrate is not significant enough to cause magnetism suppression at the interface. Although the symmetry is broken at interfaces, this effect leads only to a local ground state and does not cause the observed suppression either. The choice of interface termination does have an effect: moderate magnetism suppression is found for SrO/MnO_2 termination. Finally, we considered the effect of oxygen vacancy segregation at the interface. In the scenarios we have tested, oxygen vacancies do not suppress the interfacial magnetism. Thus, a complicated mechanism is needed to explain the suppressed magnetism at $La_{0.7}Sr_{0.3}MnO_3/SrTiO_3$ interfaces.

[1]Work supported by the Division of Materials Sciences and Engineering, BES, U.S. DoE., Computations were performed at NERSC.

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Date submitted: 11 Nov 2011 Electronic form version 1.4