Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Study of Electron Distribution and Magnetism at the Relaxed $SrTiO_3/LaAlO_3$ Interface SOHAM GHOSH, EFSTRATIOS MANOUSAKIS, Florida State University — The presence of a two-dimensional electron gas (2DEG) at the interface between two insulators $SrTiO_3$ and $LaAlO_3$ makes it an interesting topic of condensed matter research. It exhibits a variety of properties such as high mobility, magnetism and superconductivity. Bandstructure calculations have linked the presence of the electon gas to polar catastrophe and oxygen vacancy, but the value of the carrier density and its distribution is a matter of debate. In the present work, we use Density Functional Theory to study the electron density distribution and the effect of ionic relaxations on the properties of the 2DEG. In order to understand the nature of magnetism, we construct localized Wannier functions from Bloch states given by DFT and use them to calculate hopping matrix elements and exchange integrals, which act as parameters in a model to understand electron-electron correlation at the interface.

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Date submitted: 15 Nov 2013 Electronic form version 1.4