Abstract Submitted
for the CAL10 Meeting of
The American Physical Society

Oxygen vacancies in lanthanum aluminate ($LaAlO_3$) JOSHUA SAYRE, NICOLA SPALDIN, University of California, Santa Barbara — Oxygen vacancies can affect the properties of an oxide in various manners such as increasing its ion or electronic conductivity, changing its lattice constant or causing dielectric breakdown. The aim of this research is to investigate structural changes and consequent changes in properties caused by oxygen vacancies in the model complex oxide, lanthanum aluminate, $LaAlO_3$. We use density functional theory within the local density approximation (LDA) and using the VASP package to calculate the structure and properties of representative oxygen vacancy profiles. We find that the presence of oxygen vacancies modifies the pattern of rotations of the oxygen octahedra. We discuss the implications of our results for understanding the correlation between epitaxial strain in oxide thin films and intrinsic defect profiles.

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Date submitted: 04 Oct 2010 Electronic form version 1.4