Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Coupled effect of Lanthanum Defects and Oxygen Vacancies in Strontium Titanate VARADHARAJAN SRINIVASAN, ELIF ERTEKIN, JEFFREY GROSSMAN, Massachusetts Institute of Technology — Strontium Titanate, a high-dielectric constant paraelectric perovskite, exhibits multiple interesting properties, including an insulator-metal transition induced by electron doping and low temperature superconductivity. Electron doping can be achieved in a variety of manners, including (1) introduction of a large concentration of Lanthanum substitutional defects for Strontium and (2) the presence of Oxygen vacancies. We have explored, via total energy electronic structure methods based on Density Functional Theory, the coupled effect of substitutional Lanthanum defects and oxygen vacancies for a variety of configurations, and find that bound vacancy-Lanthanum pairs result in even larger increase in the carrier concentration than the individual defects alone. Strong electron localization around Oxygen atoms is observed in systems that are Oxygen deficient; these defect states lie near the Fermi level. When both Lanthanum defects and Oxygen vacancies are present, the localized defect states are pushed below the Fermi level, resulting in an even larger increase in carrier concentration.

Elif Ertekin
Massachusetts Institute of Technology

Date submitted: 20 Nov 2009 Electronic form version 1.4