Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

First principles study of $LaGaO_3/MgAl_2O_4$ (001) polar interfaces[1]

ALEJANDRO REBOLA, PETER ZAPOL, JEFFREY EASTMAN, Argonne National Laboratory, SERDAR OGUT, University of Illinois at Chicago — Materials with high oxygen ion conductivity have been the center of much attention due to both fundamental interest and technological applications. One of the most remarkable ionic conductors and an excellent candidate for future solid oxide fuel cells is $LaGaO_3$ (LGO), as it exhibits very high ionic conductivity when doped with Sr or Mg. To achieve enhanced ionic transport in this system, where oxygen vacancies (V_O) are the dominant carriers, we propose a negatively charged interface as a way of inducing a V_O enrichment layer. In this study, the interface is comprised of LGO and the spinel $MgAl_2O_4$, both of which exhibit nominally charged (001) planes. We consider an interface where the $(GaO_2)^{1-}$ layer of LGO is in contact with the $(AlO_2)^{1-}$ layer of the spinel. Such negatively charged interfaces require compensating defects, providing a strong driving force for enhancing the V_O concentration, and hence, the in-plane ionic conductivity in the space charge region adjacent to the boundary. We report results from first-principles calculations which provide information on the structure and relative stability of these polar interfaces, compensation mechanisms, and defect formation energies as a function of distance from the interface.

[1]Supported by the Office of Basic Energy Sciences, Division of Materials Sciences, U.S. Department of Energy, under Contract No. DE-AC02-06CH11357

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Date submitted: 11 Nov 2011 Electronic form version 1.4