Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Prediction of a switchable two-dimensional electron gas at KNbO3/ATiO3 (A = Sr, Ba, Pb) interfaces YONG WANG, MANISH NIRANJAN, SITARAM JASWAL, EVGENY TSYMBAL, University of Nebraska, Lincoln NE, USA — The demonstration of a quasi-two dimensional electron gas (2DEG) at the $(LaO)^{+}/(TiO_2)^{0}$ interface in $LaAlO_3/SrTiO_3$ heterostructure has fuelled intense research activity in recent years. The 2DEG has a high carrier mobility and electron density that are promising for applications in all-oxide electronic devices. For such applications it is desirable to have the ability to control the properties of the 2DEG by external stimulus, e.g., by an electric field. In this study we use density functional calculations to explore a ferroelectric $KNbO_3/SrTiO_3$heterostructure for this purpose. The polar discontinuity at the $(NbO_2)^{+}/(SrO)^{0}$interface in $KNbO_3/SrTiO_3$ heterostructure is similar to that at the $(LaO)^{+}/(TiO_2)^{+}$ interface in $LaAlO_3/SrTiO_3$ heterostructure. Our results suggest that a 2DEG is created at the $(NbO_2)^{+}/(SrO)^{0}$interface due to the electronic reconstruction with properties strongly determined by the orientation of the electric polarization. We further explore the formation of 2DEG at the interfaces of all ferroelectric $KNbO_3/BaTiO_3$ and $KNbO_3/PbTiO_3$ heterostructures and its dependence on polarization orientation. Finally, we discuss how the properties of 2DEG in aforementioned heterostructures are influenced by the compensation of polarization charges by free carriers, rendering it switchable.

Siraram Jaswal
University of Nebraska, Lincoln NE, USA

Date submitted: 21 Nov 2008 Electronic form version 1.4