

The Department of Physics and Astronomy  
Presents Research Seminar Speaker

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Time: 3:00-4:00 p.m.

Location: MB 0.302

## Emerging Phenomena in Functional Oxide Heterostructures

Multifunctional oxides (MO) are functional materials exhibiting more than one ferroic response. MO can store and release electrical, magnetic, and mechanical energy, which makes them useful as sensors, actuators, as well as memory elements. However, the coupling of even two ferroic responses *i.e.*, switching of ferroelectric order leading to commensurate changes in magnetic order is typically very weak in bulk materials. On the other hand, multifunctional oxide structures, such as epitaxially grown heterojunctions and superlattices do provide a pathway to coupling, and enable ‘designer’ polarization, strain, and magnetization effects. When combined with monolithic integration with semiconductors this technology may lead to highly integrated oxide-based electronics. I will review our theoretical studies of several functional oxide structures. First I will discuss the two-dimensional electron gas at the SrTiO<sub>3</sub>/LaAlO<sub>3</sub> interface recently reported by Hwang and others (A. Ohtomo and H. Y. Hwang, *Nature* **427**, 423 (2004)). Our calculations suggest that a complex balance of the crystal field, Jahn-Teller effect, lattice dynamics and internal electric field results in the robust electrostatic doping for carefully chosen thickness of the polar oxide. I will then show how this electrostatic doping could be extended to a ferromagnetic oxide such as EuO. Because the conduction band in EuO is spin split, one can expect introducing the spin polarized charge at the interface of EuO with a polar oxide such as LaAlO<sub>3</sub>. Another exciting concept is combining magnetic oxides with semiconductors (A. Posadas, J.-B. Yau, C. H. Ahn, et al., *Appl. Phys. Lett.* **87**, 171915 (2005)). I will describe the spin dependent Schottky barrier at the GaN/YMnO<sub>3</sub> interface. YMnO<sub>3</sub> is a very interesting material in its own right, and I will discuss how the improper nature of the ferroelectric transition in this oxide may lead to stabilizing single domain ferroelectricity in a thin film. I will then briefly describe robust magnetoelectric coupling in tri-color superlattices comprised of a ferromagnetic metal, a normal metal and a ferroelectric. All calculations are done within density functional theory. To achieve correct band gap values for SrTiO<sub>3</sub>, EuO and YMnO<sub>3</sub> we use the LDA+U approximation. For EuO we apply a Hubbard correction within the GGA (GGA+U) to the localized 4f states.

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