

MAR08-2007-007570

Abstract for an Invited Paper
for the MAR08 Meeting of
the American Physical Society

First-principles modeling of functional oxides-semiconductor interfaces¹

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Search is ongoing for new classes of materials and structures based on complex oxides. One important example is the multiferroics which combine ferromagnetism or antiferromagnetism and ferroelectricity in a single phase. The coexistence, and occasionally the coupling of the two order parameters, has opened new opportunities for multifunctional applications. A promising route for practical applications is to employ thin films and multilayered structures, the properties of which can be readily manipulated at the nanoscale. Epitaxial multiferroic films are currently being developed through integration with semiconductors. Despite the progress in synthesis and experimental characterization, the roles of the interface phenomena, including strains, chemistry, etc., on the ferroelectric and magnetic properties of multiferroic thin films is not fully understood and difficult to differentiate experimentally. In this talk we illustrate the utility of theoretical methods based on density functional theory in understanding these technologically relevant structures. We describe examples of oxide-semiconductor interfaces based on YMnO_3 on GaN that have been synthesized recently and show how interfacial spins behave differently from those in the bulk. The interfacial effects lead to an intriguing behavior of the band offsets. We also discuss our ongoing investigation of electric field doping interfaces.

¹Research in collaboration with Alex Demkov, Jaekwang Lee (University of Texas) and Craig Fennie (Argonne National Laboratory). Work at U. Texas was supported by Office of Naval Research Grant No. N000 14-06-1-0362.