MAR12-2011-001042

Abstract for an Invited Paper
for the MAR12 Meeting of
the American Physical Society

First principles insights into electronic, magnetic, and dynamic effects at and across oxide interfaces[1]

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The recent experimental capacity to create high quality epitaxial oxide/oxide interfaces has opened new avenues for research and provides examples of novel materials properties that emerge at the interfaces and in some cases only exist at the interfaces. Furthermore, a coherent, high-quality interface allows degrees of freedom in the two materials to be coupled to each other across the interface thereby creating artificial multi-functional materials systems. Ab initio theoretical approaches can provide key understanding of these complex systems as they can directly describe the interfacial chemical and structural effects on the electronic properties without assumptions or empirical parameters that are derived from bulk properties. Here, we will provide recent examples from our work showing how the presence and structure of the interface can modify the electronic, magnetic, or transport properties. For example, at a ferroelectric/manganite interface we see how the ferroelectric polarization couples to and strongly modifies the magnetism in the manganite. Another example involves dynamic coupling across an insulator/manganite interface where structural fluctuations in the insulator modify the conductivity in the manganite. In part, we will be focusing on the types of structural distortions present at such interfaces, how they are different from or non-existent in the bulk, and which type of distortions create uniquely interfacial phenomena.

[1]Primary support from NSF DMR MRSEC 0520495 and partially from NSF CNS 08-21132.