

# Electronic Structure of the Oxide Interfaces $\text{LaMnO}_3/\text{SrMnO}_3$ , $\text{LaAlO}_3/\text{SrTiO}_3$ , and $\text{CaMnO}_3/\text{CaRuO}_3$ : Carrier Density, Orbital Ordering, and Magnetism

Sashi Satpathy

*Department of Physics, University of Missouri, Columbia, MO 65211*

Our recent theoretical results on the electronic structure for several oxide interfaces of current interest will be summarized. We will focus on three interfaces, viz.,  $\text{LaMnO}_3/\text{SrMnO}_3$ ,  $\text{LaAlO}_3/\text{SrTiO}_3$ , and  $\text{CaMnO}_3/\text{CaRuO}_3$ . For the SMO/LMO, we show how strain affects the orbital ordering and magnetism, explaining results obtained in recent experiments. Also, a very interesting result is our prediction of a completely spinpolarized 2DEG at the  $\text{SMO}/(\text{LMO})_1/\text{SMO}$  delta-doped structure arising because of the double exchange. This is the 2D counterpart of a half-metallic system in 3D. A key puzzle for the LAO/STO interface has been the origin of the carrier density, viz., that while the "polarization catastrophe" argument predicts a density of  $3 \times 10^{14}$  electrons per unit cell, transport measurements have yielded a much smaller carrier density  $\sim 1-2 \times 10^{13}$ . Our detail density-functional study shows that some of the carriers may be localized and not participate in transport, suggesting a way to resolve this puzzle. Finally, we will touch upon the CMO/CRO interface, where we show that the leaked electrons from the metallic CRO side to the insulating CMO side causes a canted magnetic state at the interfacial CMO layer, consistent with the small ferromagnetic moment found in several experiments.

1. B. R. K. Nanda, S. Satpathy, and M. Springborg, *Phys. Rev. Lett.* **98**, 216804 (2007).
2. B. R. K. Nanda and S. Satpathy, "Effects of Strain on Orbital Ordering and Magnetism at the Perovskite Oxide Interfaces," *Phys. Rev. B* (submitted).
3. B. R. K. Nanda and S. Satpathy, "Two Dimensional Spin-Polarized Electron Gas at the Oxide Interfaces," *Phys. Rev. Lett.* (submitted).
4. Z. Popovic, S. Satpathy, and R. M. Martin, "On the Origin of the 2DEG Carrier Density at the  $\text{LaAlO}_3/\text{SrTiO}_3$  Interface," Z. Popovic, S. Satpathy, and R. M. Martin, *Phys. Rev. Lett.* (submitted).
5. Z. S. Popovic and S. Satpathy, *Phys. Rev. Lett.* **94**, 176805 (2005); S. Thulasi and S. Satpathy, *Phys. Rev. B* **73**, 125307 (2006); P. Larson, Z. Popovic, and S. Satpathy, *Phys. Rev. B* (2008) In press.