MAR05-2004-002688

Abstract for an Invited Paper
for the MAR05 Meeting of
the American Physical Society

**Electronic Reconstruction in Correlated Electron Heterostructures**

SATOSHI OKAMOTO, Department of Physics, Columbia University

Understanding of surface/interface properties of correlated electron materials is an important scientific question and is necessary for possible devices utilizing these materials. As a first step, we focus on the "charge leakage" between the different materials inspired by a recent experiment by Ohtomo *et al.*[1] We present the following theoretical studies of heterostructures comprised of a Mott insulator and a band insulator; (1) Hartree-Fock analysis of a realistic three-band model for a heterostructure between $LaTiO_3$ and $SrTiO_3$, the structure grown and measured by Ohtomo *et al.*,[2] (2) Dynamical-mean-field approximation analysis of a simplified single-band Hubbard model heterostructure.[3] In each case, the heterostructure is defined by placing charge +1 at La sites (charge difference between $La^{3+}$ and $Sr^{2+}$ ions), and the long-range Coulomb repulsion between conduction (Ti $d$) electrons is treated by Hartree approximation. We show that spin/orbital orderings in thin heterostructures are generically different from the bulk and that the interface region, $\sim 3$ unit cell wide, is always metallic. Prediction for photoemission experiments are made to show how the electronic properties change as a function of position through the interface. Optical conductivity measurements are proposed to investigate the nature of orderings and quasiparticle subbands. We also give general discussion of the correlated electron surface/interface problem. This work has been done in collaboration with Andrew J. Millis, and is supported by JSPS, NSF DMR 0338376 and DOE ER46169. [1]Ohtomo et al., Nature **419**, 378 (2002). [2]Okamoto and Millis, Nature **428**, 630 (2004), and Phys. Rev. B **70**, 195120 (2004). [3]Okamoto and Millis, Phys. Rev. B (in press), cond- mat/0407592.