Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

First-principles study of the band offset at the anatase $TiO_2/SrTiO_3$ (001) interface ALEXANDER DEMKOV, HOSUNG SEO, CHANDRIMA MITRA, The University of Texas at Austin — Band offsets at the interface of two oxides have recently attracted considerable attention in the context of the high-k dielectric gate stack in field effect transistors. The problem is also important in oxide heteroepitaxy. Recently, Chambers et al. reported that using the x-ray photoelectron spectroscopy no valence band offset is found between anatase TiO_2 (001) and $SrTiO_3$ (001). In this talk we describe the electronic structure at the $TiO_2/SrTiO_3$ (001) interface. We calculate the valence band offset to be 0.94 eV in the Schottky limit and 0.76 eV when the oxides are brought in contact, in apparent contradiction with experiment. A careful analysis of the electronic structure evolution from the bulk region of $SrTiO_3$ to the interface and through anatase all the way to the surface allows us to clarify the experimental results. We compare local density approximation results to those obtained with the GW method.

Hosung Seo
The University of Texas at Austin

Date submitted: 19 Nov 2010 Electronic form version 1.4