Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Density-functional modelling of electron energy-loss spectra for $LaAlO_3/SrTiO_3$ quantum well MIRI CHOI, LINGYUAN GAO, The University of Texas, QIAN HE, ALBINA BORISEVICH, Oak Ridge National Laboratory, ALEXANDER A. DEMKOV, The University of Texas — $LaAlO_3/SrTiO_3$ quantum wells (QW) are grown S by molecular beam epitaxy (MBE). The conduction band alignment is investigated using electron energy loss spectroscopy (EELS). We model the EELS spectrum using first-principle calculations. To account for the core-hole effect, the Z+1 approximationis adopted. Site-projected unoccupied p and d densities of states (pDOS) are extracted and compared with the experimental O K and Ti L edges that correspond to 1s to 2p and 2p to 3d transitions, respectively. Results fro bulk $LaAlO_3$ (LAO) and $SrTiO_3$ (STO) are discussed first and then the quantum well case is analyzed. We investigate the orbital character of the conduction band states in a QW. We find that in LAO/STO QW, there are evanescent Ti-originated states in the LAO layer and elate them with the peak at EELS front edge.

Alex Demkov
The University of Texas

Date submitted: 28 Jan 2016 Electronic form version 1.4