Contribution ID: **60** Type: **Poster**

Electronic and optical properties of LaAlO3/SrTiO3 superlattices: interface charge density, Fermi surfaces, and optical reflectivity spectra

Monday, 23 July 2012 20:00 (2 hours)

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We present calculations of the charge density profile, Fermi surface topology, and reflectivity spectra of the electron gas at the LaAlO3/SrTiO3 interface. The calculations are based on a self-consistent Hartree/RPA approximation and a tight binding parametrization of the band structure. The subband occupancy is studied as a function of polar discontinuity and dielectric constants. The number of occupied xy bands changes significantly whereas for all reasonable dielectric constant profiles only one yz and one xz bands are occupied for polar discontinuity larger than a critical value depending on dielectric constant profiles. These yz and xz band give dominant contributions to the long-distance tail of the interface charge. The optical reflectance and ellipsometry angle are calculated including optical phonon of SrTiO3. The results are compared with experimental data.

Support: DOE ER-046169

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Session Classification: Poster Session 1

Track Classification: Correlated Physics