

Abstract Submitted  
for the MAR17 Meeting of  
The American Physical Society

**GW Calculations of Bulk and Few-layer SnO<sup>1</sup>** YABEI WU, Shanghai University and State Univ of NY - Buffalo, WEIWEI GAO, WEIYI XIA, State Univ of NY - Buffalo, WEI REN, Shanghai University, PEIHONG ZHANG, Shanghai University and State Univ of NY - Buffalo — Layered structure tin monoxide (SnO) has emerged as a promising materials for a variety of applications ranging from batteries to optoelectronics. Recently, few-layer field effect transistors (FETs) using the tetrahedral (layer-structure) SnO material have been fabricated successfully recently [1]. The carrier mobility is shown to be as good as that of other 2D FETs [1]. We have carried out quasiparticle (QP) calculations within the GW approximation to understand the electronic properties of bulk and few-layer SnO. Density functional theory within the local density approximation (LDA) or generalized gradient approximation (GGA) predicts a semimetallic band structure. Upon including the self-energy effects, the QP band gap is 0.75 eV, in good agreement with experiment. We will also discuss the layer-dependence of the QP properties of SnO. [1] Saji, Kachirayil J., et al. *Advanced Electronic Materials* (2016).

<sup>1</sup>This work is supported in part by the National Natural Science Foundation of China (Nos. 11274222, 11628407, 51672171). Work at UB is supported by the NSF under Grant Nos. DMR-1506669 and DMR-1626967.

Yabei Wu  
Shanghai University and State Univ of NY - Buffalo

Date submitted: 06 Nov 2016

Electronic form version 1.4