Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Quasiparticle band structures and interface physics of SnS and GeS BRAD MALONE, School of Engineering and Applied Sciences, Harvard University, EFTHIMIOS KAXIRAS, School of Engineering and Applied Sciences, Harvard University and Department of Physics, Harvard University — Orthorhombic SnS and GeS are layered materials made of earth-abundant elements which have the potential to play a useful role in the massive scale up of renewable power necessary by 2050 to avoid unmanageable levels of climate change. We report on first principles calculations of the quasiparticle spectra of these two materials, predicting the type and magnitude of the fundamental band gap, a quantity which shows a strong degree of scatter in the experimental literature. Additionally, in order to evaluate the possible role of GeS as an electron-blocking layer in a SnS-based photovoltaic device, we investigate the band offsets of the interfaces between these materials along the three principle crystallographic directions. We find that while the valence-band offsets are similar along the three principle directions, the conduction-band offsets display a substantial amount of anisotropy.

Brad Malone
School of Engineering and Applied Sciences, Harvard University

Date submitted: 07 Nov 2012 Electronic form version 1.4