Abstract Submitted
for the NWS11 Meeting of
The American Physical Society

Optical and electronic properties of potential solar absorber Cu_3PSe_4 DAVID H. FOSTER, VORRANUTCH JIERATUM, ROBERT KYKYNESHI, DOUGLAS A. KESZLER, GUENTER SCHNEIDER, Oregon State University — We report theoretical investigations of the electronic and optical properties of semiconductor Cu_3PSe_4. Diffuse reflectance spectroscopy measurements indicate a band gap of 1.40 eV. Our calculations using the Heyd-Scuseria-Ernzerhof (HSE) hybrid functional and *GW*-type approximations agree well with the experimental atomic structure and band gap, and reveal that the band gap is direct. The calculated optical spectrum is similar to GaAs in the visible region, with $\alpha > 5\times10^4$ cm^{-1} for $\lambda < 630$ nm. We conclude that the optical properties of Cu_3PSe_4 are within the desired range for a photovoltaic solar absorber material. Of importance to material prediction (*in silico* chemistry), the local density and generalized gradient approximations (LDA/GGA) are found to cause significant error in both the HSE band gap (using HSE with ion positions relaxed in LDA/GGA) and the *GW* band gap (using *GW* with fixed LDA/GGA quasi-particle wavefunctions). We attribute this to the different degrees to which HSE and LDA/GGA find the first conduction band states to be anti-bonding (P-s/Se-p*) in character.

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Date submitted: 13 Sep 2011 Electronic form version 1.4