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Structure, stability, and defect analysis of potential solar absorber Cu_3PSe_4 DAVID H. FOSTER, JASON M. VIELMA, GUENTER SCHNEIDER, Oregon State University — The semiconductor Cu_3PSe_4 has recently been established to have a direct band gap of 1.4 eV and exhibit p-type conductivity [Applied Physics Letters, 99, 181903 (2011)]. Here we present density functional theory (DFT) and post-DFT results regarding the structure, stability, and dopability of Cu_3PSe_4. We a find a strong coupling between the electronic band gap and the atomic structure, clearly caused by the strong P-Se antibonding character of the conduction band. Using the Heyd-Scuseria-Enzerhof hybrid functional and *GW* approximation methods, we find that structural relaxation using standard DFT is not sufficiently accurate to be used as input to static, post-DFT electronic structure calculations. We use the generalized gradient approximation (GGA) and the GGA+*U* method to show a thermodynamically stable low temperature region. We calculate the formation enthalpies of intrinsic and extrinsic defects in order to understand the observed p-type behavior and to examine n-type doping mechanisms.

David Foster
Oregon State University

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