Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Structure band-gap correlations in semiconductors: Implications for computational band gap prediction GUENTER SCHNEIDER, DAVID H. FOSTER, Oregon State University — Large scale structure prediction for novel materials requires computationally inexpensive lattice relaxation methods, which are typically based on density functional theory (DFT) using a semi-local approximation for the exchange-correlation functional. These methods provide structural parameters accurate to within a few percent, but cannot predict band-gaps. Band-gap calculations, require much more computationally expensive methods such as hybrid functionals or the GW approximation. Such an accuracy-tiered method fails dramatically for Cu3PSe4. When the generalized gradient approximation (GGA) is used to relax the lattice and ions, band-gaps calculated using both the single shot GGA+GW method and the Heyd-Scuseria-Ernzerhof (HSE) hybrid functional method are a full 0.5 eV lower than the band gaps calculated for the unrelaxed, experimental structure. The GW and HSE methods predict accurate band gaps only when used with the correct experimental structure. We show that in Cu3PSe4, the calculated band-gap depends strongly on the P-Se bondlength, which can be explained by the P-Se* anti-bonding character of the lowest conduction band state. We show this effect for different lattice relaxation methods including recently developed meta-GGAs.

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Date submitted: 15 Nov 2013 Electronic form version 1.4