Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Searching Stable CuxS Structure for Photovoltaic Application
QIANG XU, BING HUANG, YUFENG ZHAO, National Renewable Energy Lab, YANGFA YAN, Department of Physics and Astronomy The University of Toledo, ROMMEL NOUFI, SU-HUAI WEI, National Renewable Energy Lab — Employing the density-functional theory (DFT) methods, we systematically search for the most energetically favorable CuxS compounds in a wide range of $1.2 < x \leq 2.0$ guided by the experimentally identified four minerals, i.e., the chalcocite (x = 2), djurleite (x = 1.94), digenite (x = 1.80), and and anilite (x = 1.75) compounds. For the chalcocite Cu2S, all its three phases have direct band gaps of 1.3-1.4 eV, with the chalcocite low phase being more stable than other two phases, i.e., the chalcocite high and the chalcocite cubic. According to our calculation, the poor durability of the Cu2S is mainly due to the energetically favorable formation of Cu vacancies. The calculated formation heat as a function of x shows that the anilite Cu1.75S is the most stable structure. Unfortunately, this material is not a good light absorber because of its metallic feature. We propose that doping of the anilite Cu1.75S with interstitial Sn atoms may result in a compound Cu1.75Sn0.125S with an optimum direct band gap of 1.37 eV. Such a material has the ability of light absorption similar to the chalcocite Cu2S.

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Date submitted: 11 Nov 2011 Electronic form version 1.4