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II-I_2-IV-VI_4 (II = Sr,Ba; I = Cu,Ag; IV = Ge,Sn; VI = S,Se): Earth-Abundant Chalcogenides for Thin Film Photovoltaics TONG ZHU, WILLIAM P. HUHN, DONGHYEOP SHIN, DAVID B. MITZI, VOLKER BLUM, MEMS Department, Duke University, BAYRAMMURAD SAPAROV, Department of Chemistry & Biochemistry, University of Oklahoma — Chalcogenides such as CdTe, CIGSSe, and CZTSSe are successful for thin film photovoltaics (PV) but contain elements that are rare, toxic, or prone to the formation of detrimental antisite disorder. Recently, the $BaCu_2SnS_{4-x}Se_x$ system has been shown to offer a prospective path to circumvent these problems.[1] While early prototypes show efficiencies of a few percent, many avenues remain to optimize the materials, including the underlying chemical composition. In this work, we explore 16 compounds II-I_2-IV-VI_4 to help identify new candidate materials for PV, with predictions based on both known experimental and computationally derived structures that belong to five different space groups. We employ hybrid density functional theory (HSE06) to explore the band gap tunability by substituting different elements, and other characteristics such as the effective mass and the absorption coefficient. Compounds containing Cu (rather than Ag) are found to have direct or nearly direct band gaps. Depending on the compound, replacing S with Se leads to a decrease of the predicted band gaps by 0.2-0.8 eV and to somewhat decreasing hole effective masses. [1] Shin *et al.*, Chem. Mater. 28, 4771 (2016).

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