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Crystal and electronic structure of quaternary chalcogenide semiconductors I_2-II-IV-VI_4 (I=Cu, Ag, II=Zn, Cd, IV=Ge, Sn and VI=S, Se, Te) SHIYOU CHEN, XIN GAO GONG, Physics Department, Fudan University, Shanghai, China, ARON WALSH, SU-HUAI WEI, National Renewable Energy Laboratory, Golden, CO — Sequential cation mutation in zinc-blende chalcogenide semiconductors, from binary to ternary to quaternary compounds, is systematically studied using first-principles calculations. Several universal trends are found for the crystal and electronic structure of the ternary and two classes of quaternary chalcogenides. We find that (i) most I_2-II-IV-VI_4 compounds are more stable in the kesterite structure, rather than the widely-recognized stannite structure; (ii) Cu and Zn layers are easy to be randomized in kesterite Cu_2ZnSnS_4 and $Cu_2ZnSnSe_4$; (iii) the band gap decreases during the mutation; (iv) the band gap of $Cu_2ZnSnSe_4$ should be around 1.0 eV, not 1.5 eV as reported in previous absorption measurements.

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