

Abstract Submitted  
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**Tin alloyed acanthite  $\text{Cu}_2\text{S}$  using cluster expansion method and their stability analysis using density functional theory<sup>1</sup>** SAJIB BARMAN, MUHAMMAD HUDA, Univ of Texas, Arlington, DR. HUDA'S GROUP TEAM —  $\text{Cu}_2\text{S}$  is a widely known semiconductor which has the potential to be used as an efficient solar absorber material. However, complex phase structures and phase instabilities due to spontaneous Cu vacancy formation are big issues which need to be addressed. Based on a recent theoretical study which has predicted acanthite like  $\text{Cu}_2\text{S}$  to be more favorable than other known crystal structures, we have used cluster expansion method to look for the most favorable tin alloyed acanthite  $\text{Cu}_2\text{S}$ . We have used density functional theory systematically to assess the stabilities of those tin alloyed acanthite  $\text{Cu}_2\text{S}$  structures. In addition, effect of Cu vacancies in Sn alloying has also been investigated.

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