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Stability study of tin alloyed acanthite Cu_2S by cluster expansion method SAJIB BARMAN, MUHAMMAD HUDA, Univ of Texas, Arlington — As a promising solar absorber material, Cu_2S is widely known in scientific community. Understanding its complex phase structures and phase stabilities are very important to apply Cu_2S as solar absorber materials. Even though recent theoretical study show that acanthite like structure of Cu_2S shows good electronic properties with suitable band gap, no experimental finding of this structure has been reported yet. Hence stabilizing this structure remains as a big challenge. In this work alloying Cu_2S with tin with a goal to stabilizing this structure will be presented. We have used density functional theory systematically to study this alloyed structures with different tin concentrations in copper layer. Alloy configurations of tin in acanthite Cu_2S are determined by cluster expansion method utilizing DFT energies. We will present our results based on these alloy configurations.

Sajib Barman
Univ of Texas, Arlington

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