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First principle investigation of the stability of silver alloyed acanthite Cu_2S. SAJIB BARMAN, MUHAMMAD HUDA, Univ of Texas, Arlington — As a potential solar absorber material, Cu_2S has proved its importance in the field of renewable energy. However, almost all the known minerals of Cu_2S suffer from spontaneous Cu vacancy formation in the structure. The Cu vacancy formation causes the structure to possess very high p-type doping that leads the material to behave as a degenerate semiconductor. This instability toward Cu vacancy formation is a vital obstacle for this material in this regard, which needs to be addressed properly. A relatively new predicted phase of Cu_2S which has an acanthite-like structure is found more preferable than the well-known low chalcocite Cu_2S. However, the Cu-vacancy formation tendency does not reduce. Alloying silver with this structure shows that Cu vacancy formation tendency can be reduced without altering its electronic property significantly. Here, we present a systematic approach within the density functional theory framework to study the stability of silver alloyed acanthite Cu_2S.

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