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Stability enhancement of solar absorber material Cu_2S by Ag alloying. SAJIB BARMAN, MUHAMMAD HUDA, University of Texas at Arlington — Cu_2S is an important solar absorber material and has great prospect in the field of renewable energy. However, this material suffers from instability due to spontaneous Cu vacancy formation and Cu diffusion in the structure. The spontaneous Cu vacancy causes the material to possess high p-type doping, which leads the material to behave as a degenerate semiconductor. This is a vital obstacle for this material to be used as an effective solar absorber material. A relatively new predicted phase of Cu_2S which has an acanthite-like structure was found to be more preferable than the well-known low chalcocite Cu_2S. However the Cu-vacancy formation tendency in this phase remained similar. We have found that alloying silver with this structure can help to reduce Cu vacancy formation tendency without altering its electronic property. The band gap of silver alloyed structure is higher than pristine acanthite Cu_2S. In addition, Cu diffusion in the structure can be reduced with Ag doped in interstitial sites. Here, we present a systematic approach within the density functional theory framework to study Cu vacancy formation tendency and diffusion in silver alloyed acanthite Cu_2S, and proposed a possible route to stabilize Cu_2S against Cu vacancy formations by alloying it with Ag.

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