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Stability enhancement of solar absorber material Cu_2S by alloying: A DFT study SAJIB BARMAN, MUHAMMAD HUDA, Univ of Texas, Arlington — Cu_2S is an important solar absorber material, which has already proved its potential in the field of renewable energy. Despite having all other important properties and being earth abundant and non-toxic, it suffers from spontaneous Cu vacancy formation, which eventually makes the material to behave as a degenerate semiconductor due to high p-type doping. As a result, the stability of the material decreases, and constricts its usages in the field of renewable energy. A relatively new phase of Cu_2S, named as acanthite-like phase is found preferable than the well-known low chalcocite phase. However, the Cu vacancy formation tendency has not improved much. We have found that alloying Ag with this new acanthite-like phase can help to reduce the vacancy formation tendency and to control the Cu atoms diffusion in the crystal. Here, we present a systematic approach within density functional theory framework to stabilize this material toward its suitable use as a renewable energy material.

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