Stability enhancement of solar absorber material Cu$_2$S by alloying: A DFT study

SAJIB BARMAN, MUHAMMAD HUDA, Univ of Texas, Arlington — Cu$_2$S 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$_2$S, 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.

Sajib Barman
Univ of Texas, Arlington

Date submitted: 21 Sep 2017

Electronic form version 1.4