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Structure prediction and electronic structure study of pristine and doped cuprous sulfide (Cu_2S)[1] PRASHANT KHATRI, Univ of Texas, Arlington, MOWAFAK M. AL-JASSIM, National Renewable Energy Laboratory, MUHAMMAD N. HUDA, Univ of Texas, Arlington — Cuprous sulfide (Cu_2S) is among the materials that have high potential of being used in solar cells, but it is highly unstable mainly due to the formation of Cu vacancies. Due to this instability of Cu_2S and mobile nature of Cu in Cu_2S, it is hard to study Cu_2S, and as a result not much is known about its structural details. A systematic theoretically understanding is necessary to utilize its potential fully in photovoltaic devices. The goal of this study is to predict the most probable structure for stoichiometric Cu_2S which is energetically favorable, and to find a mechanism to stabilize it against the formation of Cu vacancy. DFT, DFT+U and DFT-Hybrid functional theory has been used in predicting the structure and studying the properties. Many different structures have been considered while performing the calculations. Acanthite like Cu_2S structure has been found to be the most favorable structure energetically. We have also studied the structures with Cu-vacancy. A detail theoretical analysis of these aspects will be presented.

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