

DFT Study of Secondary Phase of Cu₂ZnSnS₄ in Solar Cell: Cu₂SnS₃

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Abstract : In CZTS films solar cell, the preferable reaction between Cu and sulfur vapor was likely to be induced by out diffusion of the bottom Cu component to the surface; this would lead to inhomogeneous distribution of the Cu component to form the Cu₂SnS₃ secondary phase and formation of many voids and crevices in the resulting CZTS film; which is also the cause of the decline in performance. In this work we study the electronic and optical properties of Cu₂SnS₃. For this purpose we used the Wien2k code based on the theory of density functional theory (DFT) with the modified Becke-Johnson exchange potential mBJ and the Hubbard potential individually or combined. We have found an energy gap 0.92 eV. The results are in good agreement with experimental results.

Keywords : Cu₂SnS₃, DFT, electronic and optical properties, mBJ+U, WIEN2K

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