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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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