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Structural, electronic and optical properties for chalcopyrite semiconducting materials: ab-initio computational study

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Abstract: Investigation of the physical properties of chalcopyrite materials using ab-initio methods have been carried out to simulate a new structure of thin-films photovoltaic cells with high conversion efficiency. The Density Functional Theory calculations have been performed using Wien2k computational package by employing the full-potential linearized augmented plane wave method. Structural and electronic properties of chalcopyrite semiconducting material Copper–Indium–Gallium–Selenium i.e. CuIn1-xGaxSe2 have been investigated using local density approximation for the exchange-correlation potential. The electronic structures and linear optical properties have been studied using both the semi-local Becke-Johnson potential and its modified form i.e. mBJ and TB-mBJ. Computational results are in good agreement with those acquired experimentally. The viability of alloys in realization of ultra-thin-film based (CIGS) solar cells with high performance has been proposed after simulation and analysis study using one of solar cell simulation tools. The studied material exhibits capability to become a promising candidate for fabrication of optoelectronic and photovoltaic devices.

Keywords : Chalcopyrite, FP-LAPW, optical properties, Thin-films solar cells, wien2k