

## **An Ab Initio Study of Delafossite Transparent Conductive Oxides Cu(In, Ga)O<sub>2</sub> and Absorbers Films Cu(In, Ga)S<sub>2</sub> in Solar-Cell**

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**Abstract :** Thin film chalcopyrite technology is thus nowadays a solid candidate for photovoltaic cells. The currently used window layer for the solar cell Cu(In,Ga)S<sub>2</sub> is our interest point in this work. For this purpose, we have performed a first-principles study of structural, electronic and optical properties for both delafossite transparent conductive oxides Cu (In, Ga)O<sub>2</sub> and absorbers films Cu(In,Ga)S<sub>2</sub>. The calculations have been carried out within the local density functional (LDA) and generalized gradient approximations (GGA) combined with the hubbard potential using norm-conserving pseudopotentials and a plane-wave basis with ABINIT code. We have found the energy gap is :1.6, 2.53, 3.6, 3.8 eV for CuInS<sub>2</sub>, CuGaS<sub>2</sub>, CuInO<sub>2</sub> and CuGaO<sub>2</sub> respectively. The results are in good agreement with experimental results.

**Keywords :** ABINIT code, DFT, electronic and optical properties, solar-cell absorbers, delafossite transparent conductive oxides

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