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An Ab Initio Study of Delafossite Transparent Conductive Oxides Cu(In, Ga)O2 and Absorbers Films Cu(In, Ga)S2 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)S2 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)O2 and absorbers films Cu(In,Ga)S2. 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 CuInS2, CuGaS2, CuInO2 and CuGaO2 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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