Compositionally induced valence-band offset at the grain boundary of polycrystalline chalcopyrites creates a hole barrier

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First-principles calculations of model grain boundaries (GBs) in $CuInSe_2$ $_2$ has, in addition, a conduction-band offset at the GB/GI interface, attracting electrons to the GBs. These features explain how polycrystalline chalcopyrite solar cells could outperform their crystalline counterparts. © *2005* A , t t t , , , , . [DOI: 10.1063/1.2132537]

Whereas the , t form of conventional semiconductors (Si, GaAs) has poor transport and electronic properties relative to their crystalline counterparts, surprisingly, polycrystalline alloys of $CuInSe_2$ (CIS; $E \approx 1.0$ eV) with CuGaSe

conventional single-crystal CIS. This model[1] of

atoms implies a pronounced affect on the metal–Se bonds there; the distance between the surface III layer and the nearest Se layer ($\delta = -0.17$ Å in both CIS and CGS) represent a very strong inward relaxation of the metal terminated layer.

(ii) t -t t , ´ ΔE_v - ´ t : We find (Fig. 1) that in ΔE_v(CGS) = 0.5 eV, whereas ΔE_v(CIS) = (0.2–0.3) eV. This is a consequence of the shorter Cu–Se bond length in CGS relative to CIS, and is reflected by the greater energetic separation of the Cu bands in CGS from its VBM than in CIS (i.e., larger ´ - repulsion compared with CIS). As a result, the removal of Cu atoms upon the creation of a polar GB surface lowers the VBM of CGS more than it does in CIS. The different positions of the Cu band in CIS and CGS are reflected also in the existence of a larger crystal-field splitting $\Delta_{CF} = \epsilon(\Gamma_{5v}) - \epsilon(\Gamma_{4v})$ 9. 9292 find