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Band bending near grain boundaries of $\text{Cu}_2\text{ZnSn}(\text{S},\text{Se})_4$ thin films and its effect on photovoltaic performance

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Abstract

Although the family of polycrystalline $\text{Cu}_2\text{ZnSn}(\text{S},\text{Se})_4$ (CZTSSe) thin films are well-known light absorber materials for photovoltaic solar cells and have been studied extensively in the past, the behaviors of their grain boundary (GB) still remain elusive. By using a combination of experimental techniques, we have systematically investigated the compositions and electronic structures of the grain interior (GI) and GB of the polycrystalline CZTS, CZTSe and CZTSSe films at nanometer scales. In particular, we have for the first time independently determined the band edge positions for both the conduction band and the valence band using scanning tunneling spectroscopy. While the composition of GB was nearly the same as that of GI for both CZTS and CZTSe films, opposite band bending behaviors near GBs were discovered for them. For CZTS, both the conduction band and valence band were found to bend

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