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Defect Segregations at Grain Boundaries of CuInSe2 and Cu2ZnSnSe4 and Its Impact on Photovoltaic Performance WANJIAN YIN, YELONG WU, University of Toledo, SU-HUAI WEI, ROMMEL NOUFI, MOWAFAK AL-JASSIM, National Renewable Energy Lab, YANFA YAN, University of Toledo — Grain boundaries (GBs) in absorber layers of polycrystalline thin-film solar cells play important roles in cell performance. In this presentation, we will review our recent results of density functional theory (DFT) study on the GB properties in solar cell materials including CuInSe2 (CIS) and Cu2ZnSnSe4 (CZTSe). We found that intrinsic GBs in these semiconductors are detrimental, probably due to the formation of deep gap states caused by wrong bonds. However, intrinsic defects and some extrinsic impurities have the tendency to segregate to grain boundaries. The segregations lead to two major effects: (1) passivating the deep defect states in the band gap by breaking or weakening the wrong bonding at GBs and (2) creating neutral hole barriers. The existence of Na_i^+ further induces the band bending and increases the hole barrier. Our results suggest benign GB properties in CIS. We further propose approaches to engineer GBs in CZTSe to improve its cell performance.

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