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First-principles study of low Σ grain boundaries in CdTe JI-SANG PARK, Natl Renewable Energy Lab, JOONGOO KANG, DGIST, JI-HUI YANG, WYATT METZGER, SU-HUAI WEI, Natl Renewable Energy Lab — Grain boundaries (GBs) play critical roles in determining physical properties of polycrystalline materials. In this study, we investigate stability and electronic structure of GBs in CdTe through first-principles density functional calculations. We consider low Σ symmetric tilt GBs including Σ3 (111), Σ3 (112), Σ5 (120), and Σ5 (130) GBs. We find that the Σ3 (111) GB is more stable than the other GBs considered in this study because it contains no dangling bonds and wrong bonds. The stability of the Σ3 GBs is independent on the chemical potential of Cd and Te whereas that of the Σ5 GBs depends on the chemical potentials. Unexpectedly, we find that the Σ5 (120) GBs are able to be more stable than the Σ3 (112) GBs, despite that the Σ3 (112) GBs have often been used as a model system to study GBs in polycrystalline thin-film photovoltaic materials. The Σ5 (120) GBs found in this study are not electrically harmful even though the GBs contain wrong bonds.

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