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Electronic Structures and Band Alignments of Mg_2(Si,Ge,Sn) Thermoelectric Materials[1] BYUNGKI RYU, Korea Electrotech Res Inst (KERI), EUN-AE CHOI, Korea Institute of Materials Science (KIMS), SUDONG PARK, Korea Electrotech Res Inst (KERI) — Mg_2Si, Mg_2Ge, Mg_2Sn, and their alloys are considered as eco-friendly and low cost thermoelectric materials. The low energy band structures are responsible for the electron-related thermoelectric transport, such as electrical conductivity, Seebeck coefficient, and electric part of thermal conductivity. Here, by using first principles density functional theory (DFT) calculations, we investigate the electronic structures and the band alignments of Mg_2Si, Mg_2Ge, Mg_2Sn. In DFT, the band gaps are severely underestimated compared to the experimental results. By adopting beyond-DFT calculations such as hybrid-DFT and many-body GW calculations, we obtain the reliable band gaps. We also calculate the band alignments using various calculation schemes. Based on the calculation results, we discuss the thermoelectric properties of inhomogeneous Mg_2(Si,Ge,Sn) materials.

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