Thermoelectric properties of \( p \)-type \( \text{Bi}_2\text{Te}_3/\text{Sb}_2\text{Te}_3 \) and \( n \)-type \( \text{Bi}_2\text{Te}_3/\text{Bi}_2\text{Te}_{3-x}\text{Se}_x \) superlattices\(^1\) MIN SIK PARK, JUN LI, A. J. FREEMAN, Northwestern U. — Thermoelectric superlattices are good candidates for obtaining high figure of merit (ZT) values. Indeed, the highest ZT of 2.4 at room temperature in \( p \)-type \( \text{Bi}_2\text{Te}_3/\text{Sb}_2\text{Te}_3 \) superlattices and the high ZT of 1.4 in \( n \)-type \( \text{Bi}_2\text{Te}_3/\text{Bi}_2\text{Te}_{2.83}\text{Se}_{0.17} \) superlattices are found.\(^2\) While it is well known that phonon-blocking and electron-transmission is a possible mechanism for the highest ZT in superlattices, the electron-transmission near the interface has not been studied much at the microscopic level. By first-principles calculations with the highly precise full-potential linearized augmented plane wave (FLAPW) method,\(^3\) the electronic structures and thermoelectric properties of bulk \( \text{Bi}_2\text{Te}_3 \), \( \text{Sb}_2\text{Te}_3 \) and \( \text{Bi}_2\text{Te}_{3-x}\text{Se}_x \) and of their superlattices \( \text{Bi}_2\text{Te}_3/\text{Sb}_2\text{Te}_3 \) and \( \text{Bi}_2\text{Te}_3/\text{Bi}_2\text{Te}_{3-x}\text{Se}_x \) are investigated and will be reported.

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