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Thermoelectric properties of p-type Bi_2Te_3/Sb_2Te_3 and n-type $Bi_2Te_3/Bi_2Te_{3-x}Se_x$ 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 Bi_2Te_3/Sb_2Te_3 superlattices and the high ZT of 1.4 in n-type $Bi_2Te_3/Bi_2Te_{2.83}Se_{0.17}$ 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 Bi_2Te_3, Sb_2Te_3 and $Bi_2Te_{3-x}Se_x$ and of their superlattices Bi_2Te_3/Sb_2Te_3 and $Bi_2Te_3/Bi_2Te_{3-x}Se_x$ are investigated and will be reported.

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[2]R.Venkatasubramanian, E.Siivola, T.Colpitts, and B. O'Quinn, Nature **413**, 597 (2001).
[3]Wimmer, Krakauer, Weinert, Freeman, Phys.Rev.B, **24**, 864 (1981).

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