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Electronic structure and band alignments of half-Heusler semiconductors[1] ABHISHEK SHARAN, ZHIGANG GUI, ANDERSON JANOTTI, Univ of Delaware — Half-Heuslers compounds with 18 valence electrons are promising materials for electronic and thermoelectric devices. However, data on basic parameters, such as their electronic structure, electron and hole effective masses, and the position of their valence and conduction bands with respect to those of other semiconductors are scarcely available. Here we explore a few members of this large family of compounds, TiCoSb and TiNiSn, which can be grown on conventional III-V semiconductors and could potentially be integrated in III-V-based devices. We present results of first-principles calculations of electronic structure and band alignments between these materials and with respect to conventional III-V semiconductors. Electronic structures are calculated using density functional theory within both the generalized gradient approximation and the screened hybrid functional HSE06. The results are discussed and compared to the available experimental data.

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