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Order, miscibility and electronic structure of $AgSbTe_2$-based thermoelectrics: a first principles study[1] SERGEY V. BARABASH, VIDVUDS OZOLINS, Univ. of California, Los Angeles — Using first-principles density-functional theory calculations and cluster expansion, we analyze the composition, atomic structure and electronic properties of $AgSbTe_2$-based thermoelectric alloys. In particular, for $AgBiTe_2$-$AgSbTe_2$ system, we predict that the alloys exhibit D4 cation order at all temperatures below melting, and are fully miscible down to the room temperature and below. The band structures of the $AgBiTe_2$ and $AgSbTe_2$ compounds are compared and the difference is found to originate in the spin-orbit interaction. We analyze the evolution of the Fermi surface topology at low hole dopings and use these results to refine the interpretation of the recent experimental measurements on naturally doped $AgSbTe_2$ samples.[2] We further discuss the energetics of native defects, and give a theoretical perspective on the miscibility and ordering in other quasi-ternary (Ag,Sb,X)Te alloys with rocksalt topology.

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[2]V. Jovovic and J.P. Heremans, Phys. Rev. B **77**, 245204 (2008).

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