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Electronic structure of defects in Mg_2Si and Cu_3SbSe_4 and their thermoelectric significance[1] S.D. MAHANTI, DAT DO, Michigan State University — Defects play an important role in the thermoelectric properties of narrow band gap semiconductors. Recently, Mg_2Si and its solid solutions with Mg_2Sn have been found to be excellent n-type thermoelectrics and have been studied extensively due to its unique feature called conduction band convergence [Liu et al., PRL 108, 166601 (2012)]. In this talk we will discuss the physics of defects in Mg_2Si and explore the possibilities of improving its thermoelectric properties by co-doping, using first principle calculation and supercell model. In addition, we will also discuss some of our results using the same approach on the nature of defects in another important thermoelectric system Cu_3SbSe_4 where the lone pairs of Sb control the nature of states near the band gap [Dat Do et al., J. Phys.: Condens. Matter 24, 415502 (2012)].

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