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Electronic structure of PbTe doped with K and Na[1] MAL-SOON LEE, S. D. MAHANTI, Michigan State University — PbTe is a well-known thermoelectric which shows excellent thermoelectric performance (for both *p*- and *n*-type) in the temperature range between ambient and 600°C. Thermopower (S) of PbTe can be enhanced with proper doping. Hermann *et al.* have found the figure of merit ZT=1.5 at 773 K with 2 % Tl doping in PbTe. They ascribe this to the enhancement of the density of states (DOS) caused by Tl-induced resonance level in the valence band. This is in agreement with the *ab initio* studies of Ahmad *et al.*, who also found an enhanced DOS associated with K defects in PbTe. Recently Androulakis *et al.* have looked for resonant states in the valence band associated with Na/K impurities in PbTe. Although they observe an increase in power factor at high temperature, they do not find any evidence of resonant states. We have reexamined this issue by carrying out detailed band structure calculations in the presence of K and Na defects in PbTe using 64-atom supercells. The question of the existence of resonant states and the origin of the enhanced DOS near the valence band maximum will be discussed.

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