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Impact of impurities on the electronic structures of thermoelectric material Mg_2Si[1] KA XIONG, SABINA SOBHANNI, RAHUL GUPTA, WEICHAO WANG, BRUCE GNADE, KYEONGJAE CHO, University of Texas at Dallas — Thermoelectric (TE) materials have attracted a lot of attention because of its capability of converting heat into electricity or vice versa. In this work, we investigate the effects of dopants in Mg_2Si, which is a promising TE material candidate. We calculate the electronic structures and stability of various dopants (Al, In, P, As, Sb, Bi, Ag, Cu, Zn, and Cd) in Mg_2Si with different charge states, using density functional theory (DFT) method with HSE functional which gives accurate band gap prediction. This DFT study helps us to gain insights on the defect states of these dopants in Mg_2Si and the mechanisms which cause the modulation of the Mg_2Si TE efficiency.

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