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Electronic structure and p-type doping of $ZnSnN_2$ TIANSHI WANG, ANDERSON JANOTTI, CHAOYING NI, Univ of Delaware — $ZnSnN_2$ is a promising solar-cell absorber material composed of earth abundant elements. Little is known about doping, defects, and how the valence and conduction bands in this material align with the bands in other semiconductors. Using density functional theory with the the Heyd-Scuseria-Ernzerhof hybrid functional (HSE06), we investigate the electronic structure of $ZnSnN_2$, its band alignment to other semiconductors, such as GaN and ZnO, the possibility of p-type doping, and the possible causes of the observed unintentional n-type conductivity. We find that the position of the valence-band maximum of $ZnSnN_2$ is 0.55 eV higher than that of GaN, yet the conduction-band minimum is close to that in ZnO. As possible p-type dopants, we explore Li, Na, and K substituting on the Zn site. Finally, we discuss the cause of unintentional n-type conductivity by analyzing the position of the conduction-band minimum with respect to that of GaN and ZnO.

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