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# Study of the Thermoelectric properties of n-type $\text{Mg}_3\text{Sb}_2$ via doping Zr and incorporating MXene

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In recent times, there has been a growing interest in thermoelectric Zintl compounds due to their excellent thermoelectric performance across various families. Among these,  $\text{Mg}_3\text{Sb}_2$ -based Zintl compounds have garnered attention as potential thermoelectric materials. However, their effectiveness is hindered by weak electrical transport properties stemming from their p-type nature. The poor electrical transport characteristics of p-type  $\text{Mg}_3\text{Sb}_2$  can be attributed to its high thermal conductivity, low hole concentration, and relatively large band gap of 1.23 eV, primarily resulting from the presence of Mg vacancies. Nevertheless, an excess of Mg can reduce these vacancies, transforming the material into an n-type compound with superior electrical transport properties, thereby making it a more promising candidate for thermoelectric applications. Consequently, n-type  $\text{Mg}_3\text{Sb}_2$ -based materials have emerged as viable options for temperatures ranging from 300 K to 773 K, owing to their high band degeneracy, low lattice thermal conductivity, low toxicity, and abundance. Among these materials, Te-doped  $\text{Mg}_{3+x}\text{Sb}_{1.5}\text{Bi}_{0.5}$  stands out as particularly promising, as the excess Mg combined with moderate Te doping enables the regulation of carrier type and concentration. Notably, Tamaki et al. demonstrated that a sample with a composition of  $\text{Mg}_{3.2}\text{Sb}_{1.5}\text{Bi}_{0.49}\text{Te}_{0.01}$  achieved a remarkable figure of merit of  $zT$  1.5 at 716 K. Our objective here is to further enhance the thermoelectric properties of n-type  $\text{Mg}_{3.2}\text{Sb}_{1.5}\text{Bi}_{0.49}\text{Te}_{0.01}$  through doping and forming a composite.

## Academic year

3rd year

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