

Supporting Information

Understanding the influence of Bi/Sb substitution on carrier concentration in Mg₃Sb₂-based materials: Decreasing bandgap enhances the degree of impurity ionization

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Supplementary Table

Table S1 The sample density (d) of $\text{Mg}_{3.175}\text{Mn}_{0.025}\text{Sb}_{1.96-x}\text{Bi}_x\text{Te}_{0.04}$ measured by Archimedes method.

| Samples | Density (g/cm^3) | Relative density (%) |
|----------|------------------------------------|----------------------|
| $x=0.48$ | 4.4 | 97% |
| $x=1.2$ | 5.03 | 95% |
| $x=1.44$ | 5.28 | 93% |

Supplementary Figure

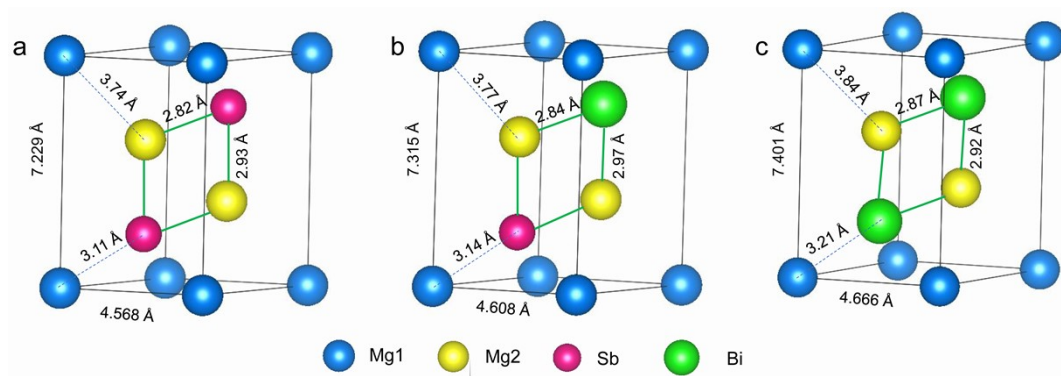


Fig. S1 The optimized crystal structures of $\text{Mg}_3\text{Sb}_{2-x}\text{Bi}_x$ ($x=0, 1$ and 2).