Electronic Supplementary Information

Improved Stability and High Thermoelectric Performance Through Cation Site Doping in n-type La-doped Mg$_3$Sb$_{1.5}$Bi$_{0.5}$

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Figure S1. Temperature dependence of Hall carrier concentration of La-doped sample (La$_x$Mg$_{3.05}$Sb$_{1.5}$Bi$_{0.5}$, $x=0.005$-0.03) and Te-doped sample (Mg$_{3.05}$Sb$_{1.5}$Bi$_{0.5}$Te$_{0.01}$).
**Figure S2** X-ray diffraction peak pattern of La-doped sample \((La_xMg_{3.05}Sb_{1.5}Bi_{0.5}, x=0.005-0.03)\). \(Mg_3Sb_2\) (ICSD-2142) is also shown for comparison. X-ray diffraction of the sample was measured at room temperature on a STOE-STADIMP powder diffractometer equipped with an asymmetrically curved Germanium monochromator (MoK\(\alpha_1\) radiation, \(\lambda = 0.70930 \text{ Å}\)). The line focused X-ray tube was operated at 50 kV and 40 mA. The sample was placed on a metallic holder and measured in reflection geometry in a rotating stage.
Table S1 Heat capacity values used to calculate thermal conductivities from diffusivity measurements. The value is obtained from a thermodynamic model curve that fits experimental measurements. Details will be published elsewhere.¹

<table>
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<tr>
<th>T(K)</th>
<th>298</th>
<th>323</th>
<th>373</th>
<th>423</th>
<th>473</th>
<th>523</th>
<th>573</th>
<th>623</th>
</tr>
</thead>
<tbody>
<tr>
<td>C_p(J/mol·K)</td>
<td>123.6</td>
<td>124.8</td>
<td>126.9</td>
<td>128.6</td>
<td>130.0</td>
<td>131.2</td>
<td>132.4</td>
<td>133.4</td>
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Reference