Electronic Supplementary Information

Improved Stability and High Thermoelectric Performance Through Cation Site Doping in n-type La-doped $Mg_3Sb_{1.5}Bi_{0.5}$

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Figure S1. Temperature dependence of Hall carrier concentration of of La-doped sample

(La_xMg_{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). Mg₃Sb₂ (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 (MoKα1 radiation, $\lambda = 0.70930$ 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

<i>T</i> (K)	298	323	373	423	473	523	573	623
$C_{p}(J/mol \cdot K)$	123.6	124.8	126.9	128.6	130.0	131.2	132.4	133.4

Reference

[1]Agne, M. T. et al. unpublished (2018).