Significantly enhanced thermoelectric figure of merit of p-type Mg₃Sb₂-based Zintl phase compound via nanostructuring employing high energy mechanical milling coupled with

spark plasma sintering

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Supplementary Information:

The XRD pattern of the bulk $Mg_3Sb_{2-x}Bi_x$ (x = 0 & 0.2) along with their different hours ball milled nanostructured counterparts (i.e. 10, 20 and 30 hr) were shown in the supplementary information. The XRD pattern for all the samples were done after spark plasma assisted sintering (SPS) reaction.



Figure S1: XRD pattern of different nanostructured materials obtained after milling of 10, 20 and 30 hrs along with their bulk counterparts.

Table ST1: shows the lattice parameter for the bulk Mg_3Sb_2 and $Mg_3Sb_{1.8}Bi_{0.2}$ with their bulk nanostructured 30 hrs ball milled counterpart respectively.

Samples	a	С
Bulk Mg ₃ Sb ₂	0.45636 nm	0.72299 nm
Nanostructured Mg ₃ Sb ₂	0.45982 nm	0.72430 nm
Bulk Mg ₃ Sb _{1.8} Bi _{0.2}	4.56666 nm	7.23542 nm
Nanostructured Mg ₃ Sb _{1.8} Bi _{0.2}	4.60319 nm	7.32222 nm