SUPPLEMENTARY INFORMATION

Enhanced Bulk Thermoelectric Performance of $Pb_{0.6}Sn_{0.4}Te$: Effect of Magnesium Doping

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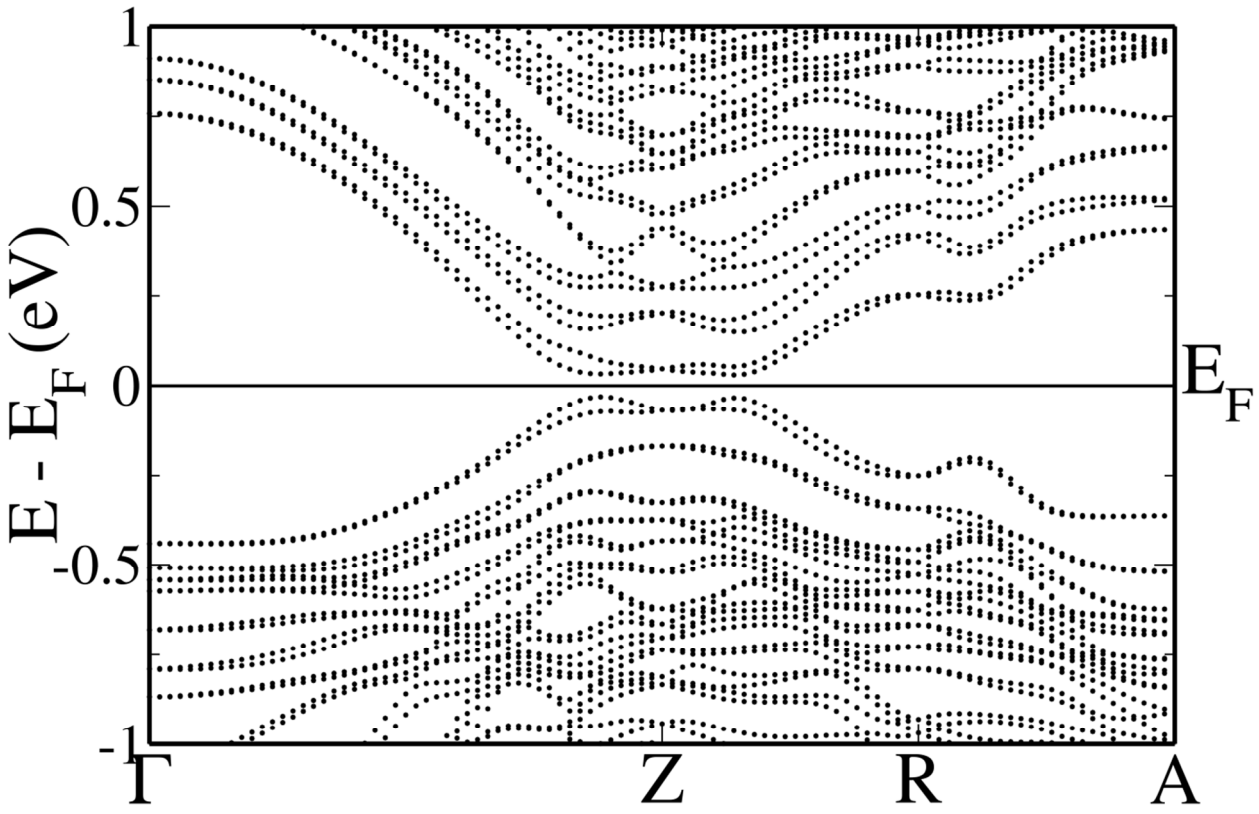

Figure S1. Electronic structure of $Pb_9Sn_6MgTe_{16}$ (D-II configuration) with Mg in zinc blende site determined using a 2×2×1 supercell.

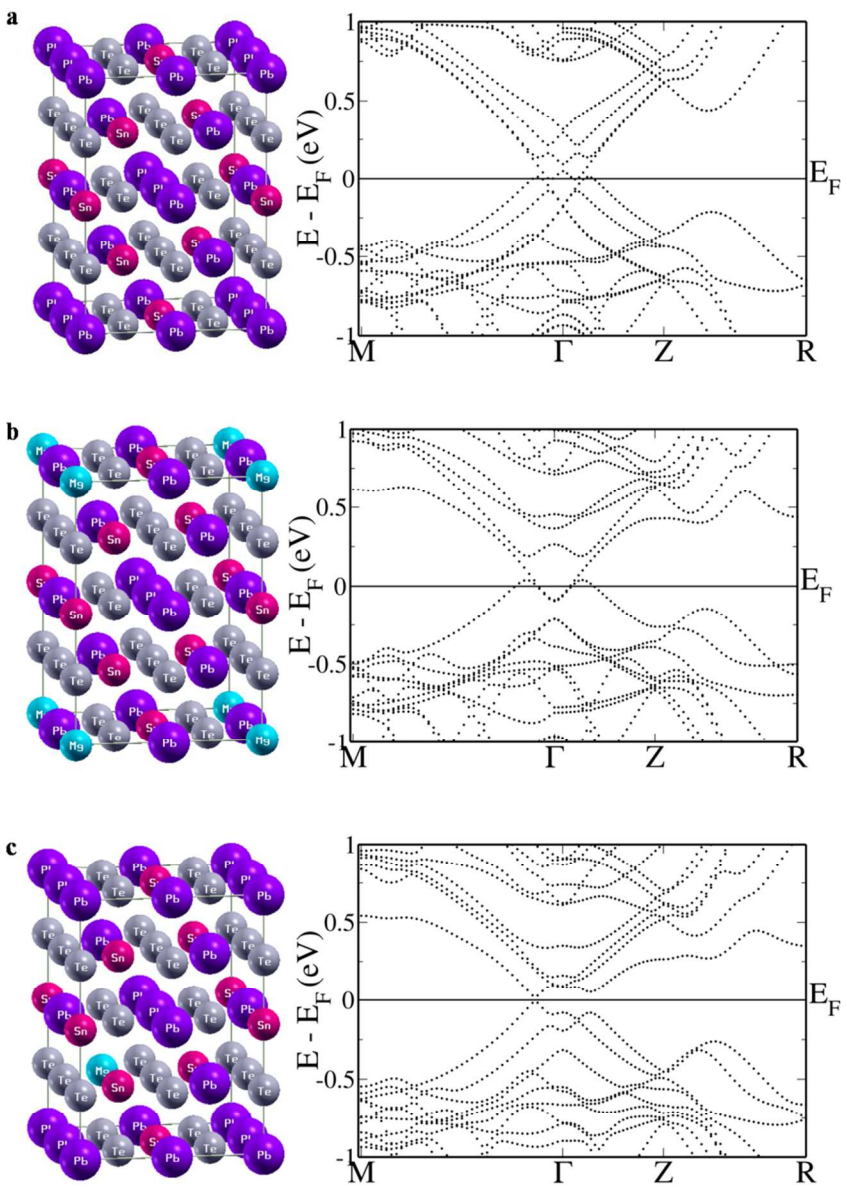

Figure S2. Crystal structures and corresponding electronic structures of a) $Pb_{10}Sn_6Te_{16}$, $Pb_9Sn_6MgTe_{16}$ b) with mirror symmetry retained and c) with breaking of local symmetry determined using $\sqrt{2}\times\sqrt{2}\times2$ supercell containing 32 atoms.

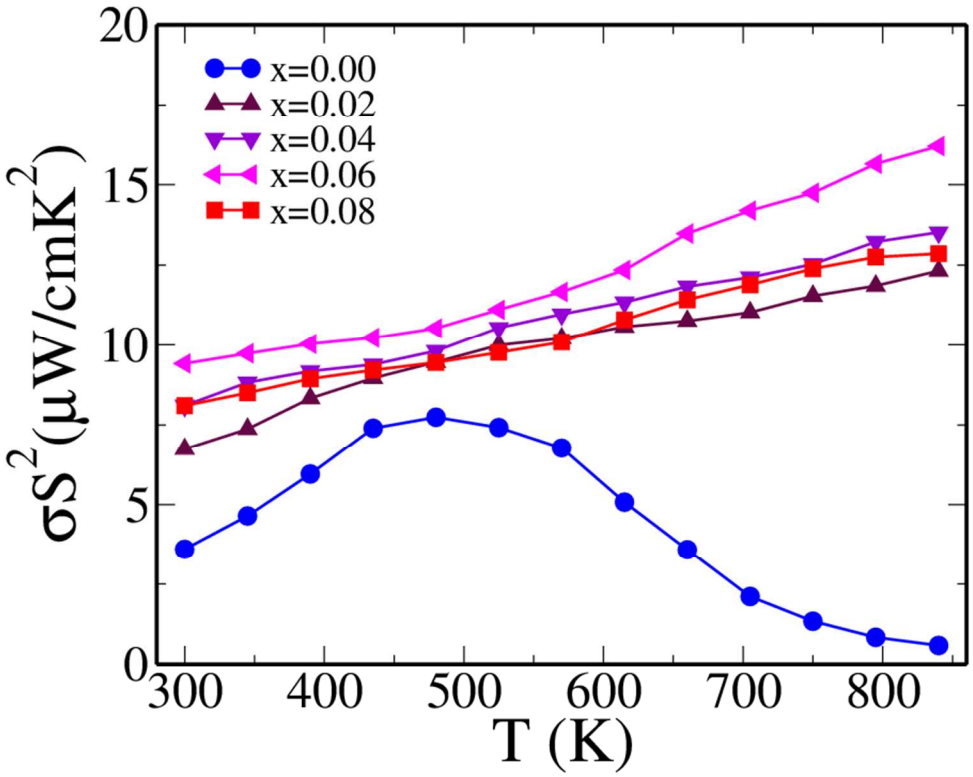

Figure S3. Temperature dependent power factor of $Pb_{0.6-x}Sn_{0.4}Mg_xTe$.