Supplementary Material

DFT based study on structural stability and transport properties of Sr3AsN: A potential thermoelectric material

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This supplementary document presents thermoelectric parameters as a function of carrier concentration at 300 and 500 K for both p and n-type Sr3AsN.

FIG. S1. Calculated: (a) Seebeck coefficient, (b) electrical conductivity, (c) electronic part of the thermal conductivity, and (d) power factor, as a function of the carrier concentration of p-type Sr3AsN.

The calculated Seebeck coefficient, electrical conductivity, electronic thermal conductivity, and power factor (PF) within a constant relaxation time of p-type Sr3AsN are shown in FIG. S1. These parameters for n-type Sr3AsN are shown in FIG. S2.



FIG. S2. Calculated: (a) Seebeck coefficient, (b) electrical conductivity, (c) electronic part of the thermal conductivity, and (d) power factor, as a function of the carrier concentration of n-type Sr3AsN.