

Supplementary material of “Strong anharmonicity and medium-temperature thermoelectric efficiency in antiperovskites Ca_3XN ($\text{X} = \text{P}, \text{As}, \text{Sb}, \text{Bi}$) compounds”

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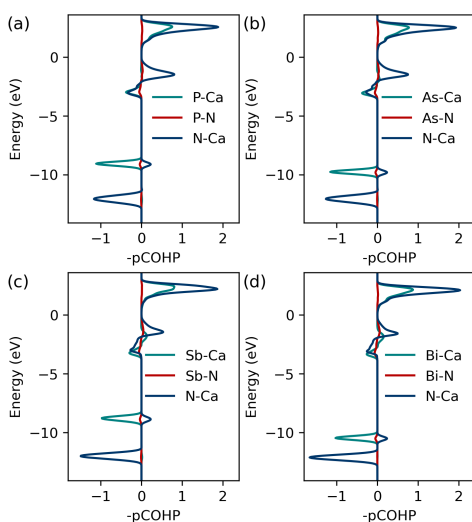


Figure 1: Crystal orbital Hamilton population (COHP) of Ca_3XN for the nearest neighbor of bonding: (a) Ca_3PN (b) Ca_3AsN (c) Ca_3SbN (d) Ca_3BiN .

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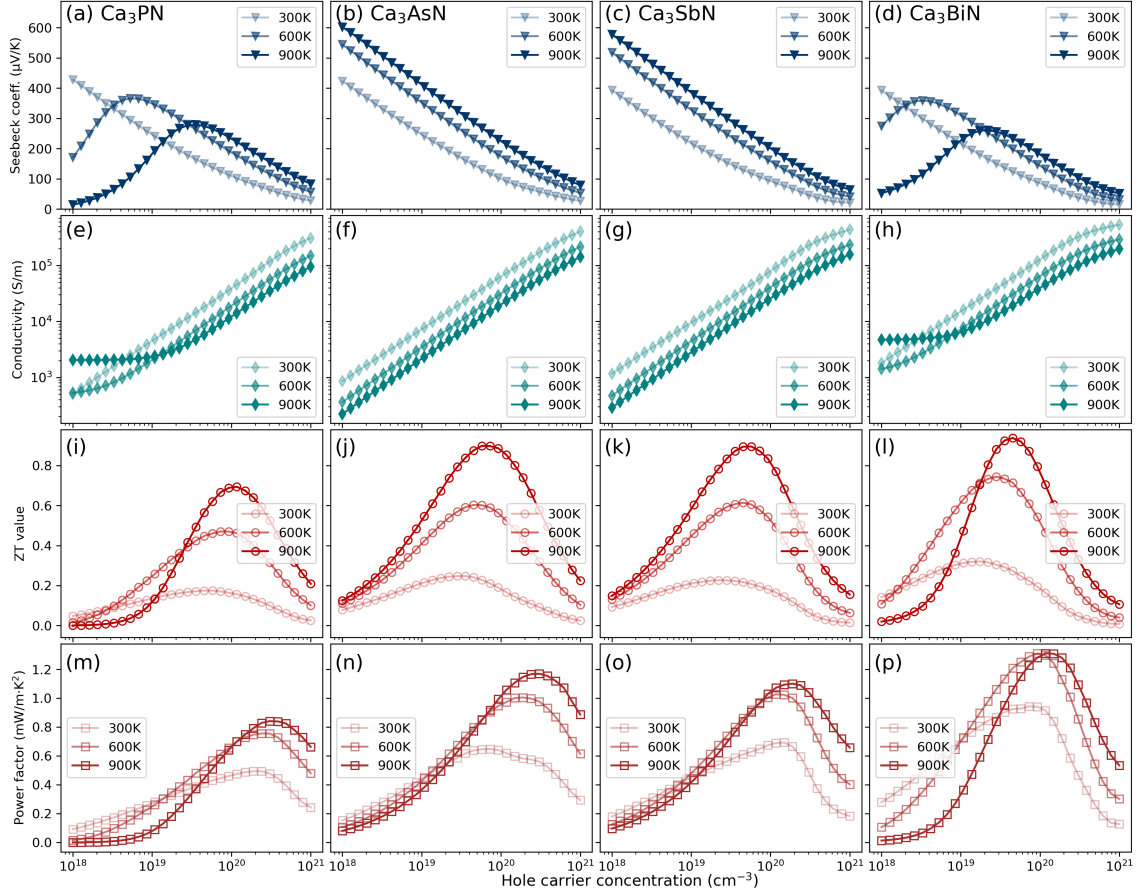


Figure 2: The p-type electronic transport parameters of Ca_3XN : (a-d) Seebeck coefficient S , and (e-h) figure of merit ZT at 300, 600, and 900 K, respectively. From left to right is: Ca_3PN , Ca_3AsN , Ca_3SbN and Ca_3BiN .