Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information for Promising thermoelectric candidate based on $CaAs_3$ monolayer: a first principles study

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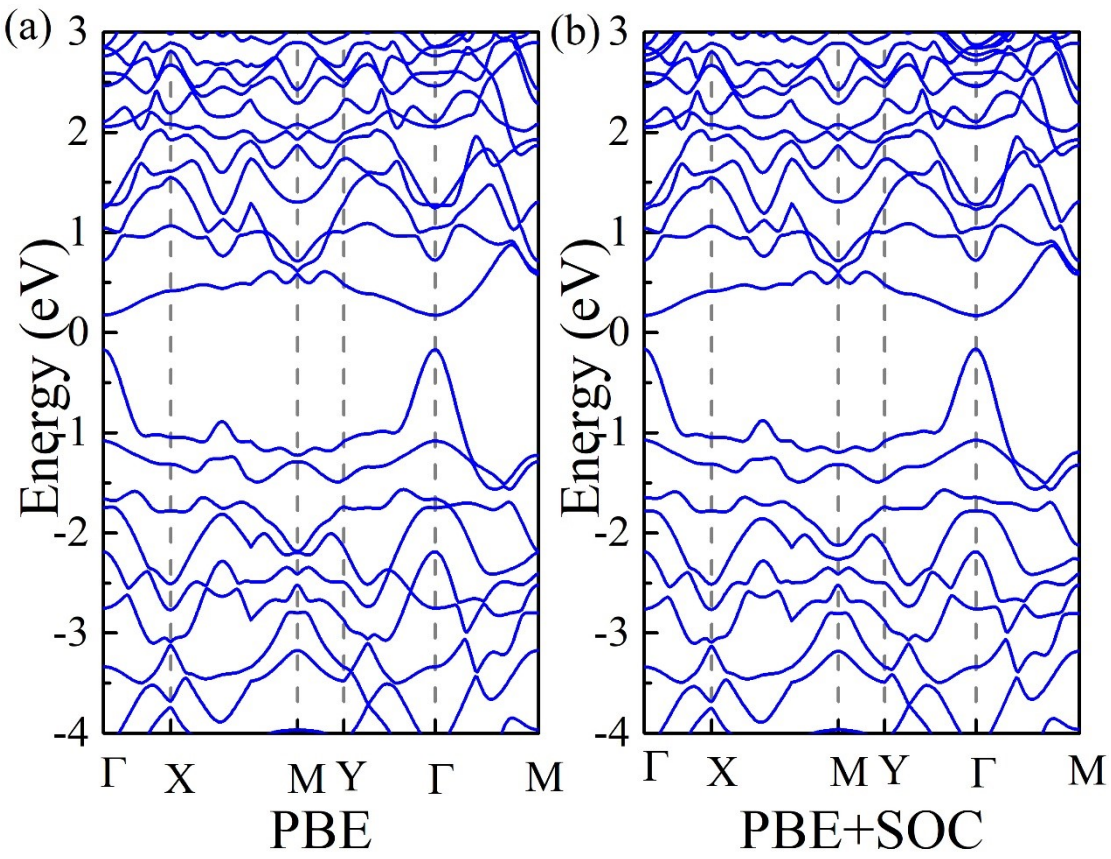

Fig. S1. The band structure of $CaAs_3$ monolayer calculated from PBE (a) and PBE+SOC (b).

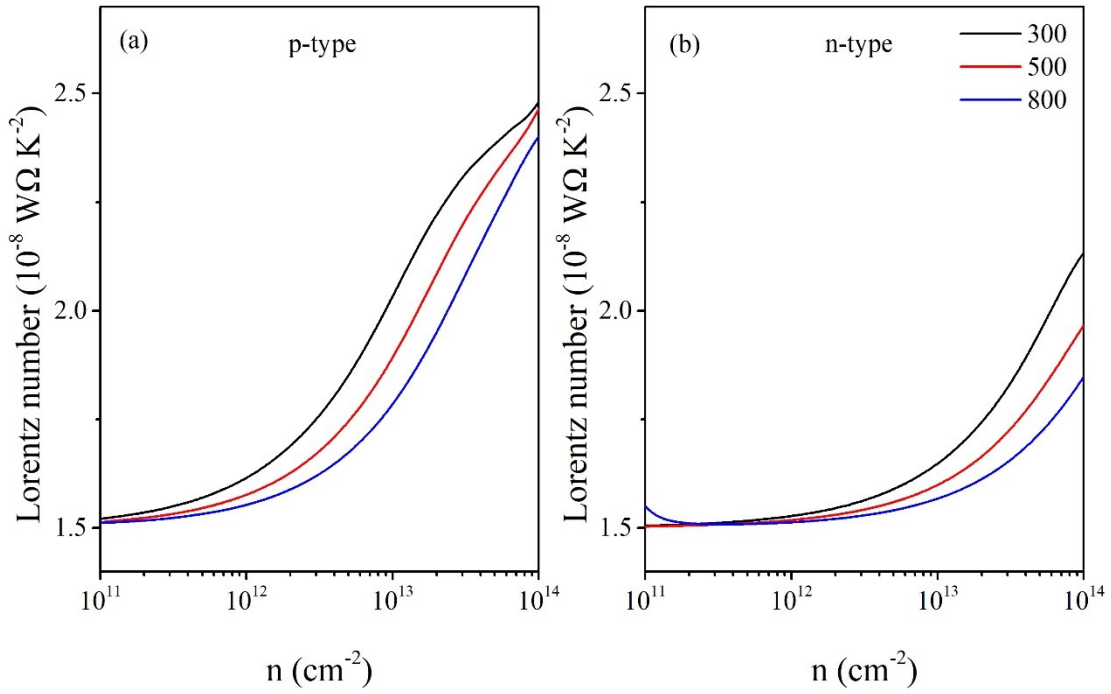

Fig. S2. Lorenz number as a function of carrier concentration (holes and electrons) at 300, 500, and 800 K. Based on the Seebeck coefficients, the Lorenz number can be

calculated by $L = 1.5 + exp[-\frac{|S|}{116}]$.