Supplementary Materials

Electronic structure and thermoelectric properties of Zintl compound $Sr_5Al_2Sb_6$ and $Ca_5Al_2Sb_6$: First-principles study

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We simulate the ZT value of $Ca_5Al_2Sb_6$ as a function of carrier concentration at 700 K without considering the anisotropy, shown as Fig. S1(b). Comparing with the experimental work from Ref. 7, shown as Fig. S1(a), we can see that the simulated ZT value agree with the experimental work, indicating that our computational method is believable.

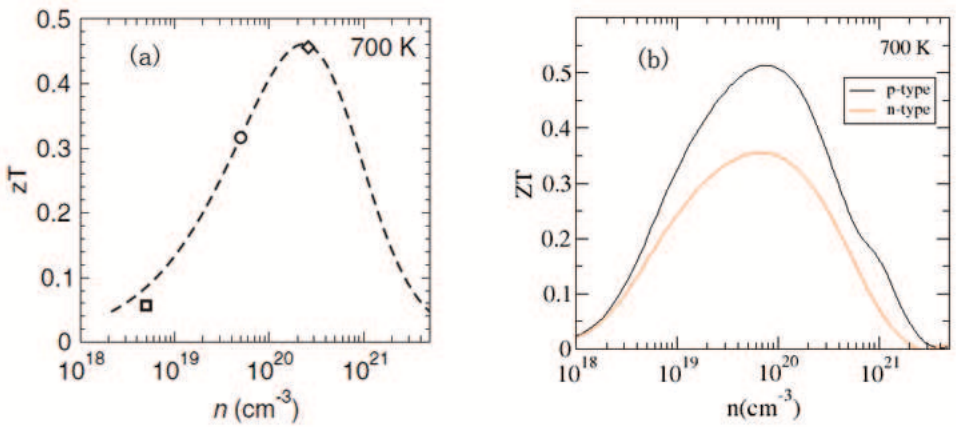

FIG. 1. (a) Experimental ZT value of $Ca_5Al_2Sb_6$ versus carrier concentration at 700 K, (b) Simulate ZT value of $Ca_5Al_2Sb_6$ versus carrier concentration at 700 K.