

Supplementary Information for

Br doping-induced evolution of the electronic band structure in dimorphic and hexagonal SnSe₂ thermoelectric materials

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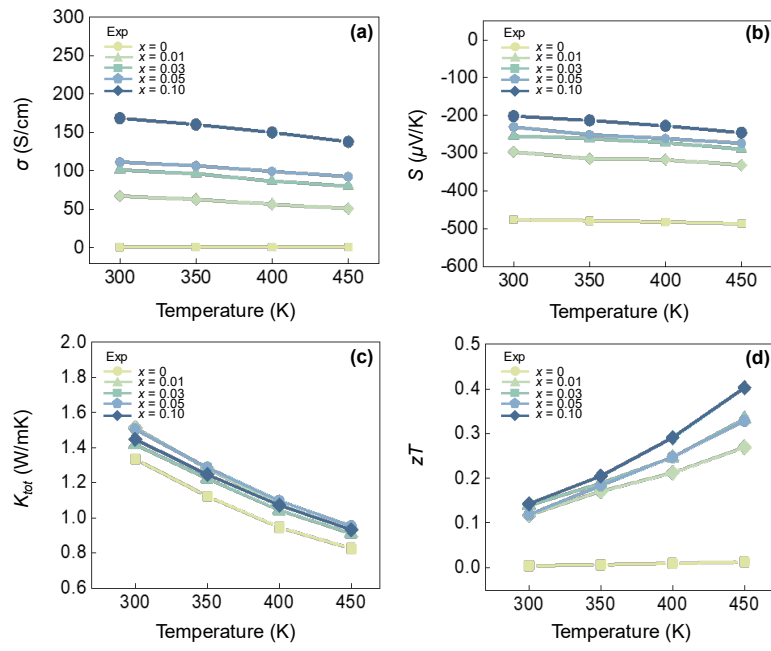


Fig. S1 Temperature-dependent (a) σ , (b) S , (c) κ_{tot} , and (d) zT of $\text{SnSe}_{2-x}\text{Br}_x$ ($x = 0 - 0.10$).¹

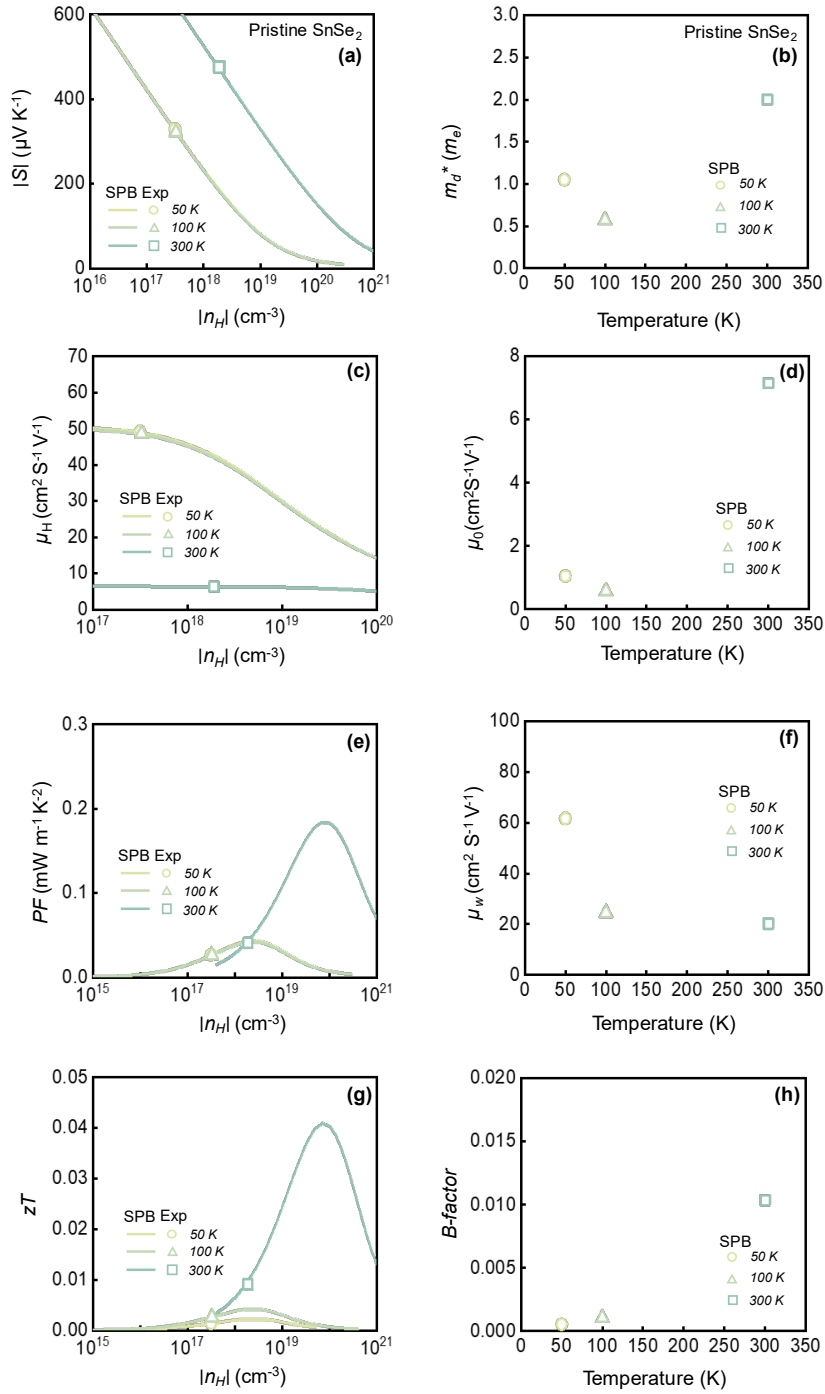


Fig. S2 (a) Calculated and experimental S as a function of n_H , (b) temperature-dependent m_d^* , (c) calculated and experimental μ_H as a function of n_H , (d) temperature-dependent μ_0 , (e) calculated and experimental PF as a function of n_H , (f) temperature-dependent μ_w , (g) calculated and experimental zT as a function of n_H , (h) temperature-dependent B -factor for pristine SnSe₂ at 50 – 300 K.²

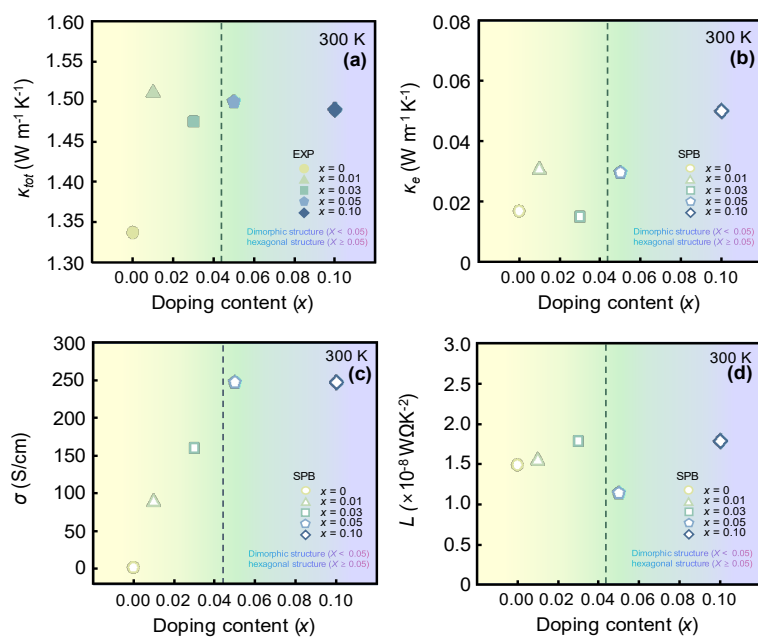


Fig. S3 (a) Experimental total thermal conductivity (κ_{tot}), (b) calculated κ_e , (c) experimental σ , and (d) calculated L for different Br doping content (x).¹

References

1. M. Liu, J. Zhang, J. Xu, B. Hu, B. Liu, K. Sun, Y. Yang, J. Wang and B. Du, *J. Solid State Chem.*, 2020, **289**, 121468.
2. J. Wang, X. Jia, S. Lou, G. Li, S. Zhou, *ACS Omega*, 2020, **5**, 12409.