Supplementary Material

Monolayer SnP_3: An excellent p-type thermoelectric material†

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Selection of K-mesh

The difference between the last two phonon q-grids was less than 5%, which indicated the convergence of the shengBTE calculation. From the figure S1, we can see that the lattice thermal conductivity gradually converges as the k mesh increases. The lattice thermal conductivity along Zigzag direction is about 5.41 W/mK with the 33 × 33 × 1 k-mesh, which is very close to 5.43 W/mK with the 35 × 35 × 1 k-mesh. Therefore, based on the test of k-mesh, we use the 35 × 35 × 1 k-mesh for our calculations.

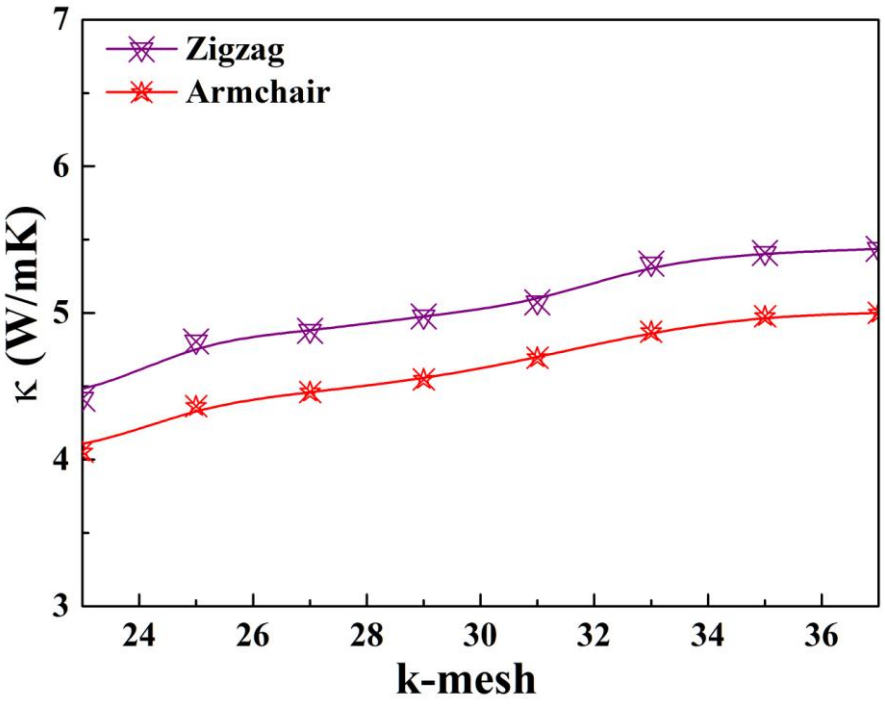

Figure S1 The lattice thermal conductivity as a function of k-mesh at 300 K.

The Lorenz number

To more accurate estimate the TE performance, the calculated Lorenz numbers are

presented in Fig. S2. Based on the Seebeck coefficients, the Lorenz number can be calculated by $L = 1.5 + \exp[-\frac{|S|}{116}]$. The values of Lorenz numbers are 2.19, 2.18, and 2.18×10^{-8} $W\Omega K^{-2}$ along armchair direction at 300, 500 and 700 K, while the corresponding Lorenz numbers are 2.22, 2.21, and 2.20×10^{-8} $W\Omega K^{-2}$ along armchair direction, respectively.

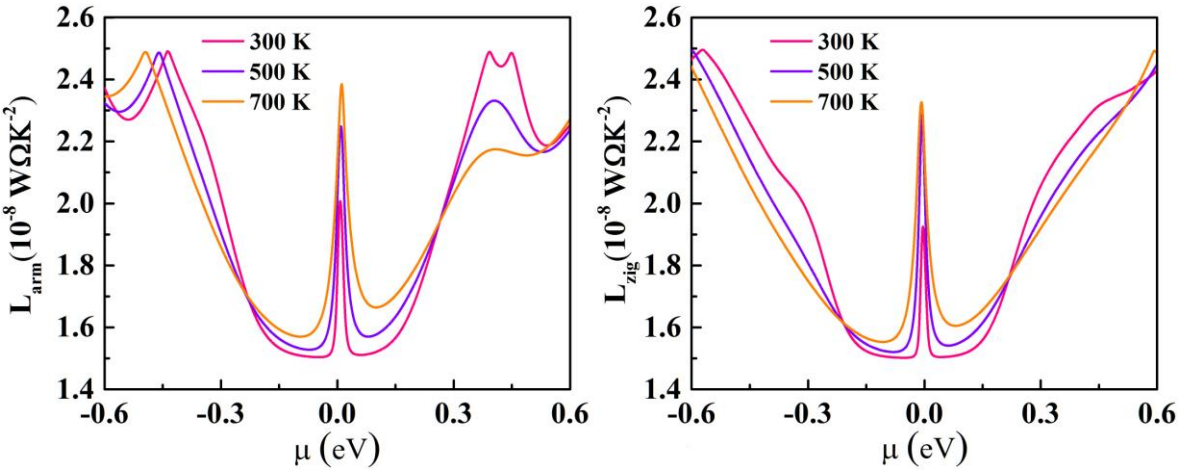

Figure S2 Lorenz number as a function of the Fermi level along armchair and zigzag directions.

The thermal stability

Based on the calculation of AIMD, one can see that the SnP_3 can remain relatively stability with slight disrupted at 700 K.

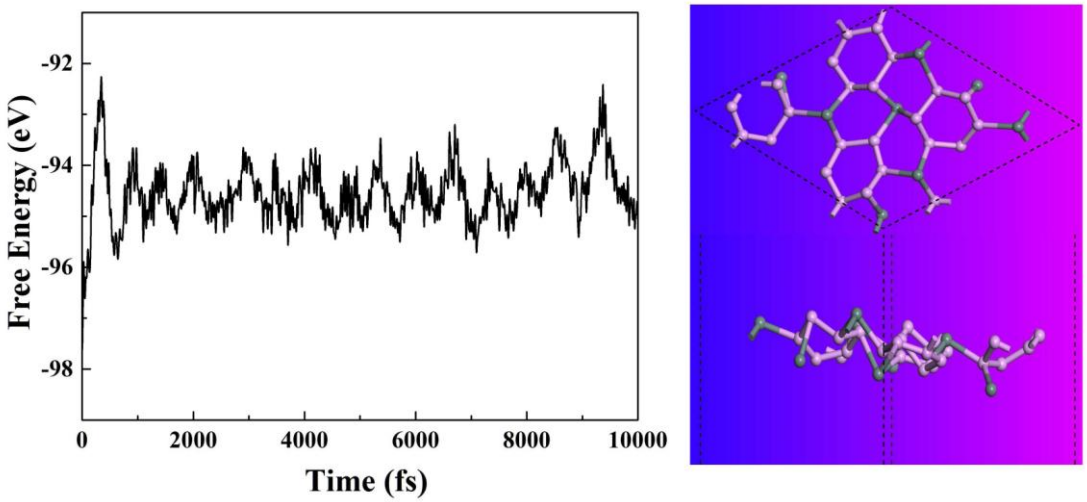

Figure S3 Variation of the free energy in the AIMD simulations at 700 K over the time scale of 10 ps.

Table S1. Crystal structure details

Compounds	Space Group	Lattice Parameters (Å)	Atom Positions (POSCAR)
SnP_3	$R\bar{3}m1$ (No. 164)	a = b = 7.37; c=20	SnP3-PBE+vdw-DF2 1.000000000 7.377063634 0.000000000 0.000000000 -3.688531870 6.388724510 0.000000000 0.000000000 0.000000000 20.00000000 P Sn 6 2 Direct 0.830957732 0.169042253 0.504903795 0.830957732 0.661915465 0.504903795 0.338084535 0.169042282 0.504903795 0.502375641 0.497624419 0.471137866 0.502375581 0.004751192 0.471137866 0.995248838 0.497624389 0.471137866 0.333333343 0.666666687 0.559637671 0.000000000 0.000000000 0.416403990