Supplementary Information (SI) for Journal of Materials Chemistry C.

Supplementary Information

Exceptionally low thermal conductivity in simple two-dimensional SiS: anomalous emergence of rattling phonon modes in non-caged materials

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S1. Convergence test

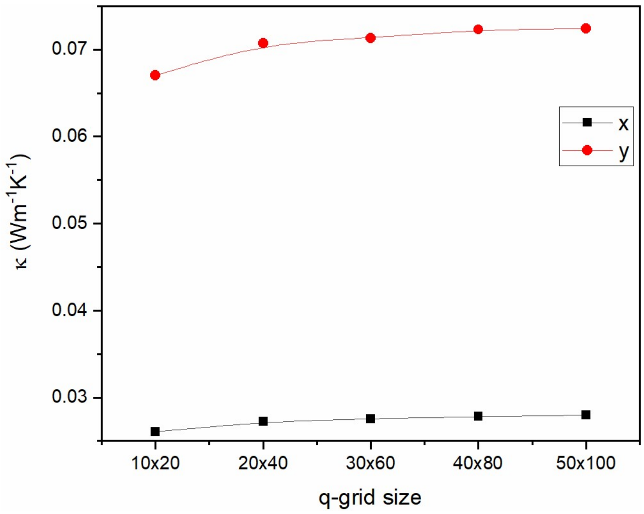

Figure S1. Convergence of thermal conductivity along the x and y direction with respect to the q-grid size.

S2. The thermal conductivity without considering the VDW interaction

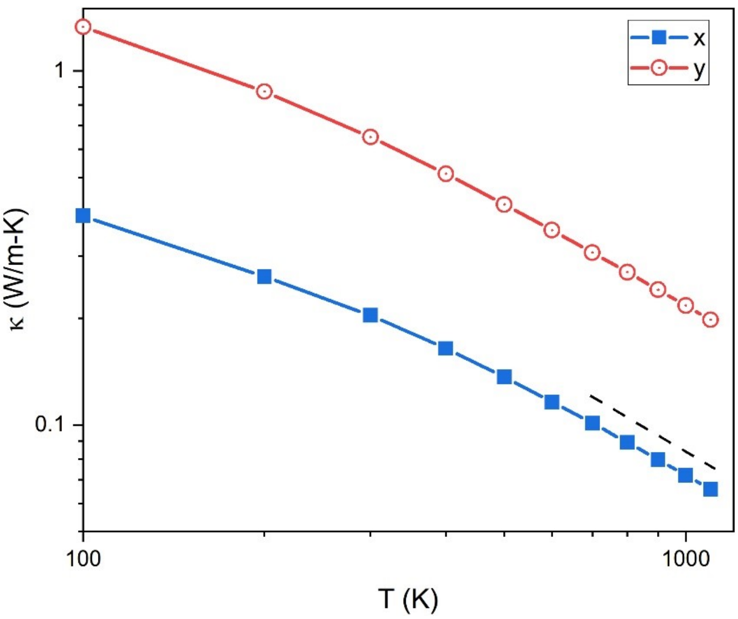

Figure S2. Thermal conductivity of 2D SiS without considering the VDW interaction

S3. Effect of four phonon scattering on thermal conductivity

We use the Fourthorder.py package to calculate the fourth-order force constants up to the second neighbor within a 3×5×1 supercell. We then solve the BTE, incorporating the four-phonon scattering processes, using a q-mesh of 20×40×1. The scattering rates for four-phonon processes are approximately two orders of magnitude smaller than those for three-phonon processes. As a result, four-phonon scattering has a minimal impact on thermal conductivity. For instance, the thermal conductivities are 0.072 $Wm^{-1}K^{-1}$ without considering four-phonon scattering, and 0.068 $Wm^{-1}K^{-1}$ when it is included.

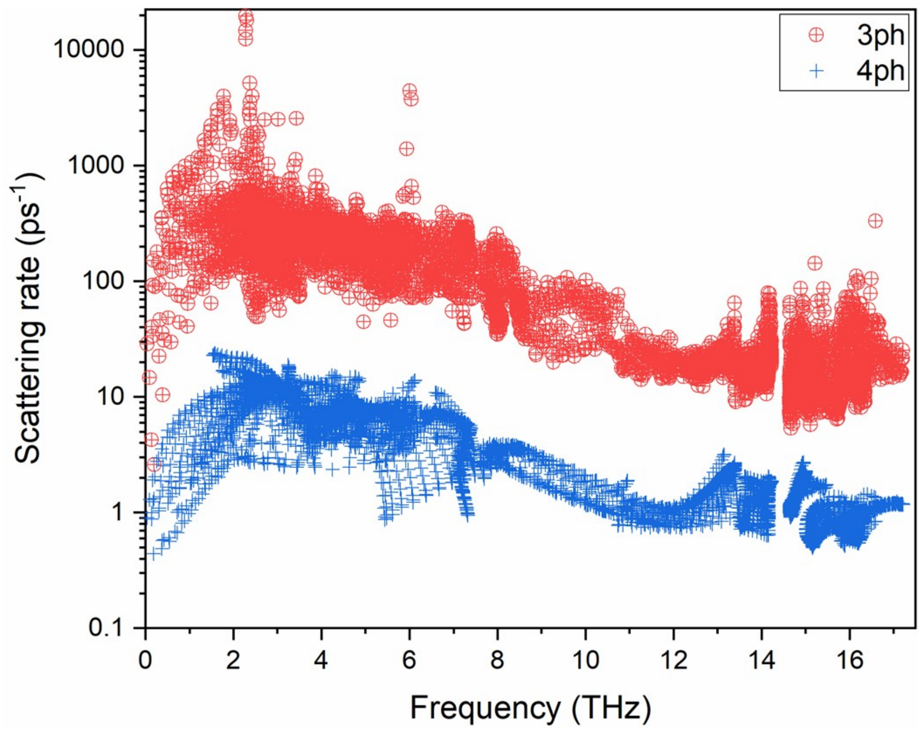

Figure S3. Scattering rates of three-phonon (3ph) and four-phonon (4ph) processes as a function of frequency.

S4. The electronic transport properties of n-type 2D SiS

Since the work by Yang et al.[1] revealed that electron carriers in 2D SiS exhibit much higher mobility than hole carriers, we focus on the electronic transport properties of n-type 2D SiS computed using BoltzTrap[2]. Figure S3 shows the ratio between electronic conductivity (σ) and relaxation time (τ), the Seebeck coefficient (S), and the power factor (PF) as a function of carrier concentration for n-type 2D SiS.

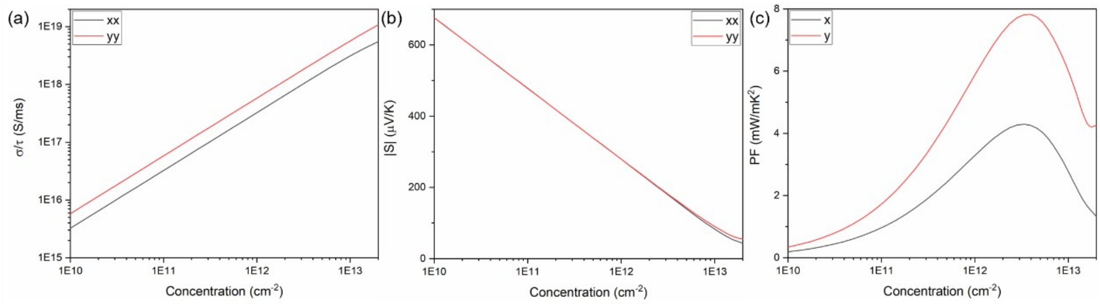

Figure S4. The σ/τ, Seebeck coefficient (S), and power factor (PF) as a function of carrier concentration for n-type 2D SiS.

References

1. J.-H. Yang, Y. Zhang, W.-J. Yin, X. Gong, B. I. Yakobson and S.-H. Wei, *Nano Lett.*, 2016, **16**, 1110-1117.

2. G. K. Madsen and D. J. Singh, *Comput. Phys. Commun.*, 2006, **175**, 67-71.