Supporting information for

Anomalous thermal transport behavior in graphene-like carbon nitride (C_3N)

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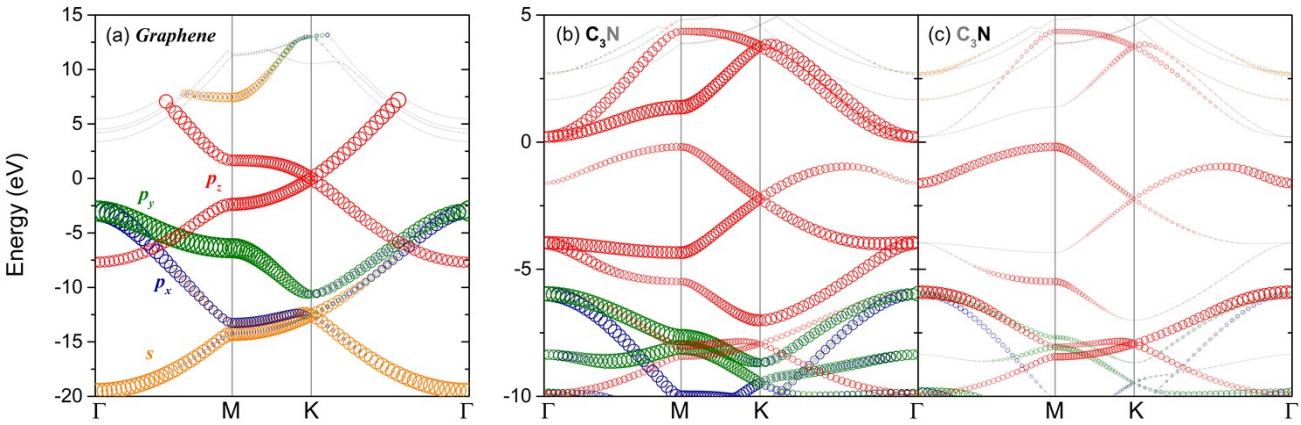

Fig. S1. The orbital projected electronic structures for (a) Graphene, (b) C atoms in C_3N, and (c) N atoms in C_3N. The relative contribution of corresponding oribitals are represented by the size of the circles

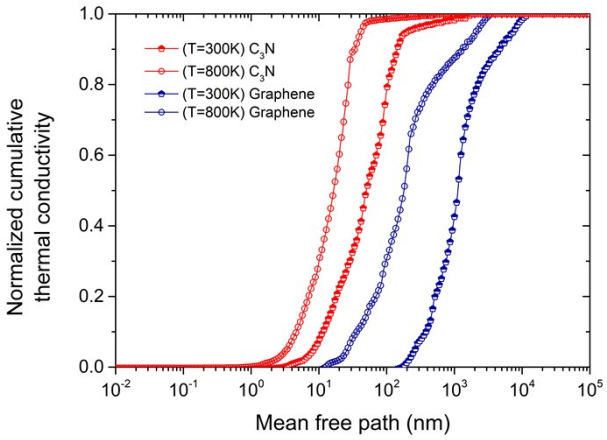

Fig. S2**.** Comparison of the normalized cumulative κ of C_3N and graphene at 300 and 800 K as a function of phonon mean free path.

To evaluate the effect of four phonons, we plotted the ratio of four-phonon scattering phase space (P_4) to three-phonon scattering phase space (P_3) as a function of frequency (Fig. S3). For BAs, it is shown that P_4 is significantly higher than P_3, which implies that four-phonon scattering dominates the phonon-phonon scattering process. In contrast, in monolayer C_3N, P_4 is smaller than P_3, which proves that three-phonon plays a dominant role in phonon-phonon scattering. In addition, the ratio of P_4 total to P_3 total for BAs and C_3N is plotted in the inset of Fig. 3 to more clearly measure the effect of four-phonon scattering in C_3N. Based on the above analysis, the behavior of the four phonons in C_3N is weak and can be ignored, which is consistent with the gapless characteristics of phonon dispersions of C_3N (Fig. 1 in the main text).

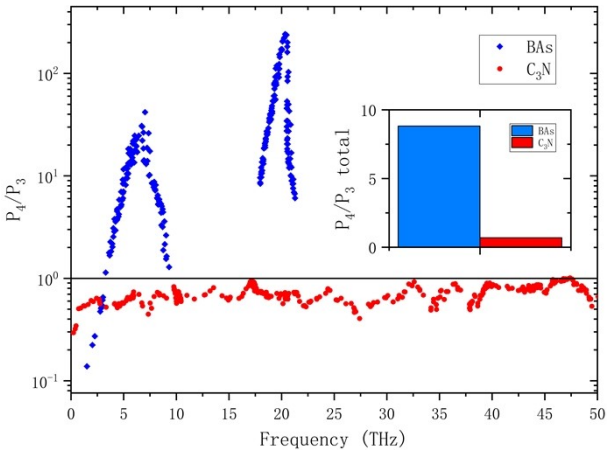

Fig. S3. The ratio of four-phonon scattering phase space (P4) to three-phonon scattering phase space (P3) for BAs and C_3N. The inset shows the ratio of P_4 total to P_3 total for BAs and C_3N.

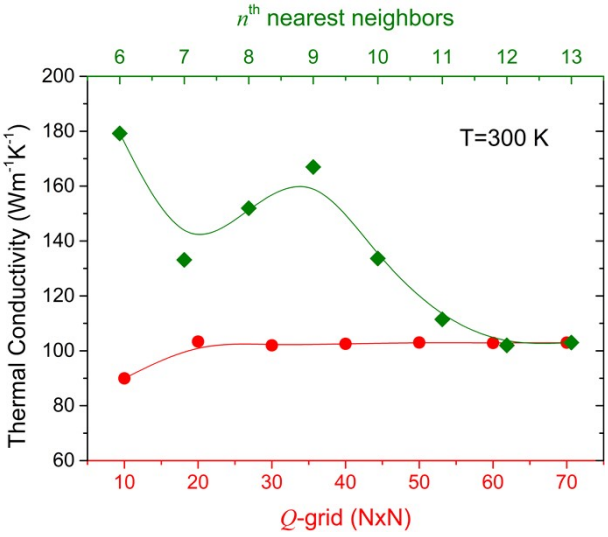

Fig. S4 The convergence test of κ with respect to the cutoff distance and Q-grid are fully conducted, based on which the cutoff distance is chosen as 7.36 Å (13th nearest neighbors) for the 3rd IFCs calculations and the Q-grid is chosen as 50 × 50 × 1 for the κ calculations.

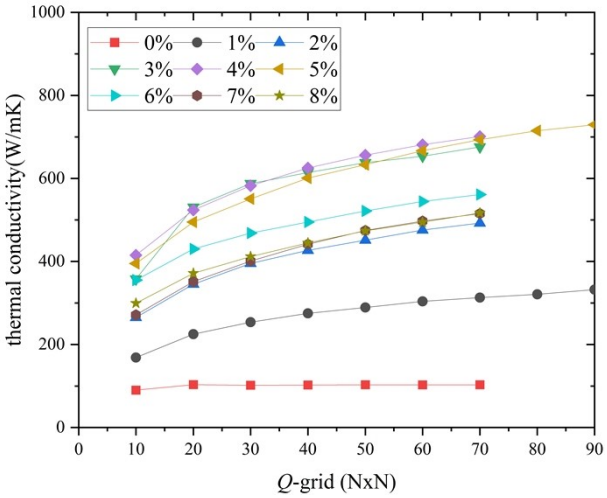

Fig. S5 Convergence test of κ in terms of Q-grid under at 1% to 8% strains.