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Supplementary Information for "Modulation of thermal conductivity, interlayer thermal resistance, and interfacial thermal conductance of C_2N"

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S1. Phonon dispersion of C_2N

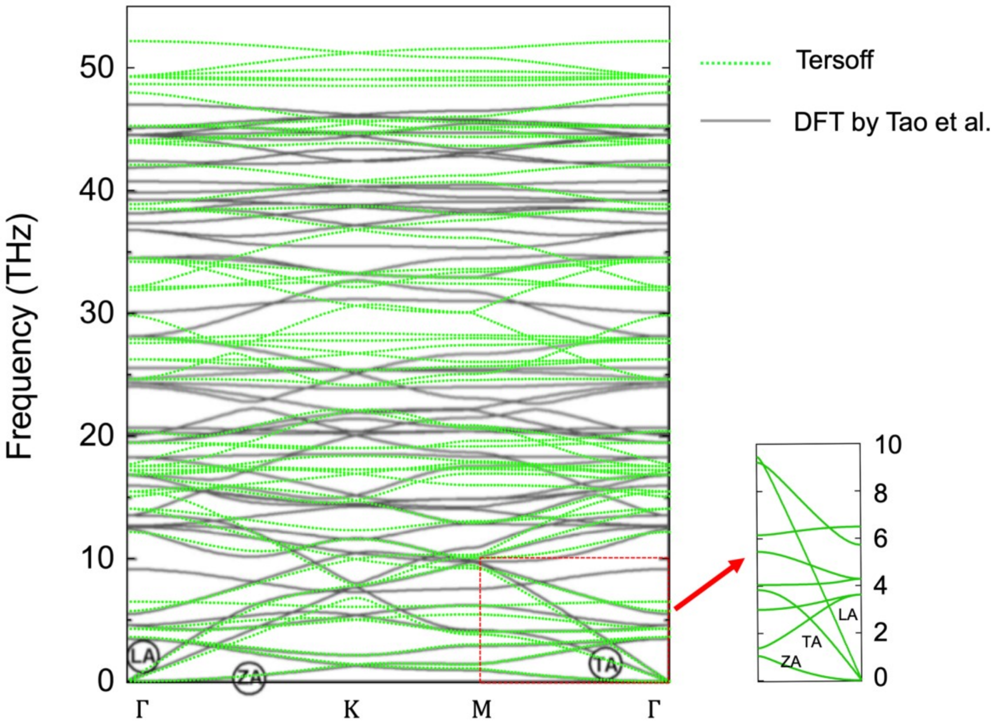

Fig.S1. Phonon dispersion of C_2N

Three acoustic branches, including the longitudinal acoustic (LA), transverse acoustic (TA), and out-of-plane acoustic (ZA) phonon mode are in agreement with the DFT results of Tao et al. As shown in the inset of Fig.S1, near the Γ point in the center of the Brillouin zone, the LA and TA modes are linearly distributed, while the ZA mode is quadratically distributed, similar to graphene.

S2. Temperature distribution in the C_2N/C-C_2N heterostructure

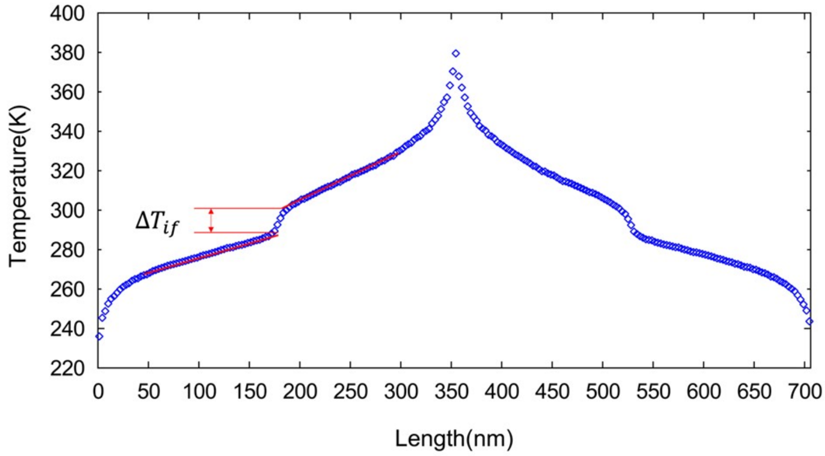

Fig. S2. Temperature distribution in the C_2N/C-C_2N heterostructure along the heat flux direction.

S3. Width effects on k_i

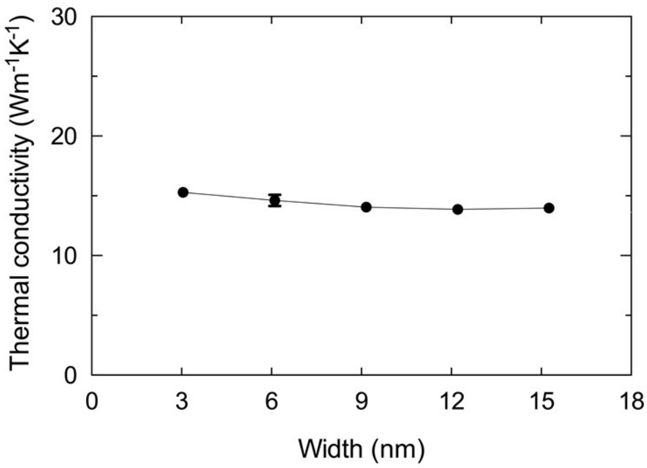

Fig.S3. The influence of model widths ranging from 3 to 15 nm on k_i

S4. Primitive cell of C_2N

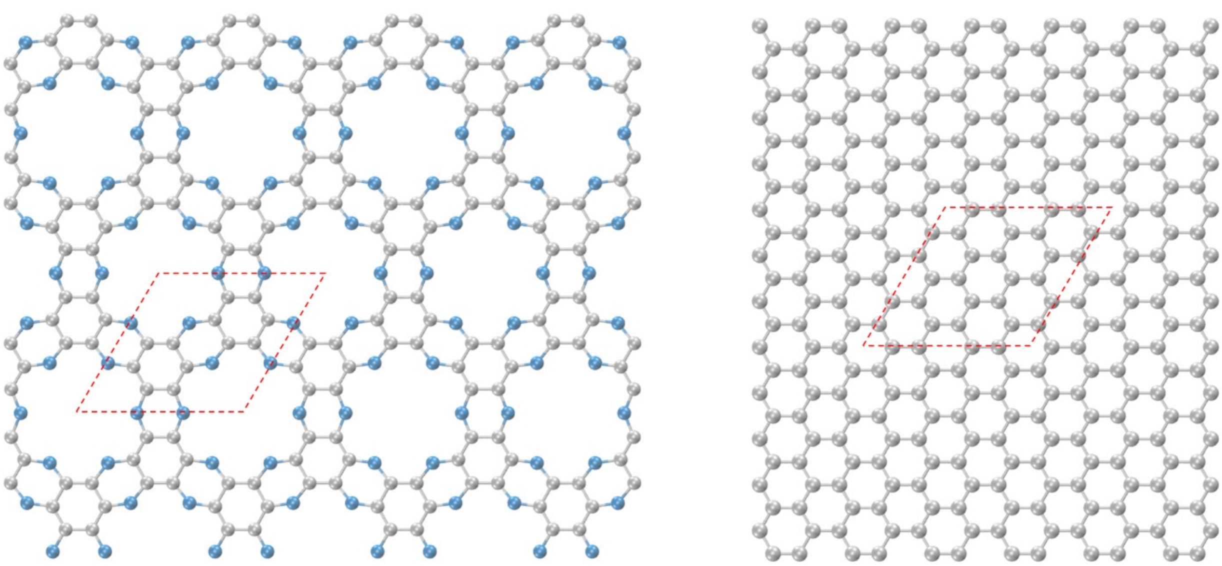

Fig.S4. Atomic structure of graphene and C_2N. The 18-atoms unit cell of C_2N and the 24-atoms unit cell of graphene are shown.

S5. Geometric optimization of models for C and N atomic defects

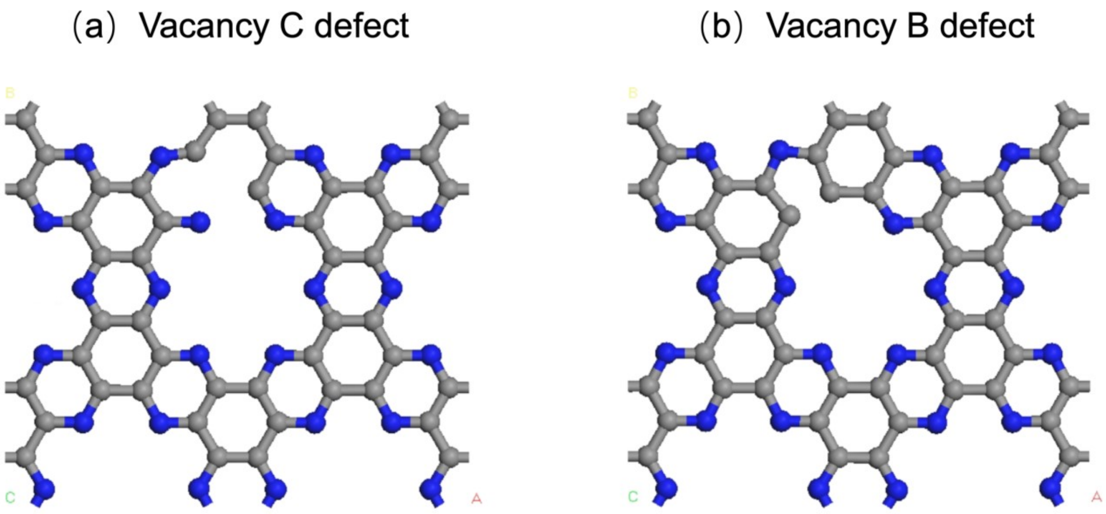

Fig.S5. Geometric optimization of C_2N with C and N defects.

DFT calculations are performed as implemented in CASTEP using the Perdew-Burke-Enzerhof generalized gradient approximation exchange-correlation functional. The energy cutoff is 400 eV.

S6. Stress-strain curve

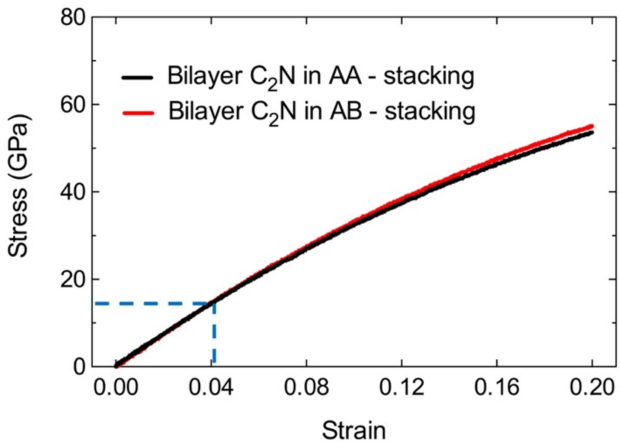

Fig. S6. Engineering stress-strain response of bilayer C_2N in AA- and AB- stacking.

S7. Stress distributions of C_2N/C-C_2N heterostructures

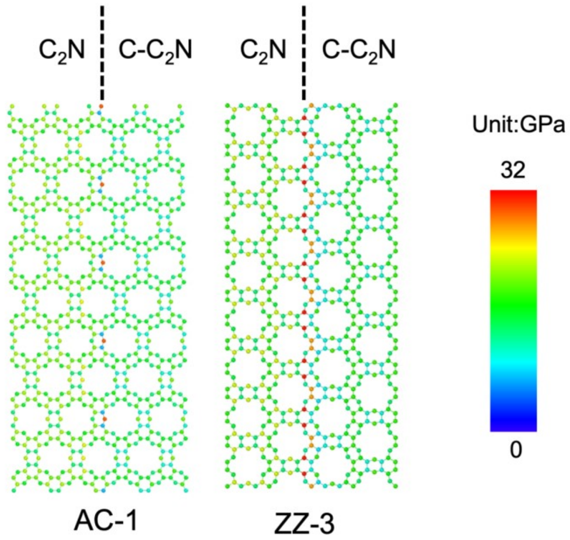

Fig. S7. Stress distributions of C_2N/C-C_2N heterostructures at the AC-1 and ZZ-3 interfaces.