Electronic Supplementary Information (ESI) for

First-principles calculations of phonon behaviors in graphether: a comparative study with graphene

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1. The list of thermal conductivities of representative 2D monolayers

Table S1. The summary of thermal conductivities of representative 2D monolayers at 300 K using first-principles calculations.

2D material	Reference	k (W m^{-1} K^{-1})
graphether	Our work	600.91 (armchair) 393.32 (zigzag)
graphene	Our work	3544.41
graphene	Peng et al.[1]	3716.6
h-BN	Lindsay et al.[2]	~520
C_2N	Ouyang et al.[3]	82.22
C_3N	Peng et al.[4]	482
C_3B	Wang et al.[5]	301
silicene	Xie et al.[6]	9.4
germanene	Peng et al.[1]	2.4
stanene	Peng et al.[7]	11.6
phosphorene	Jain et al.[8]	36 (armchair) 83.5 (zigzag)

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MoS_2	Gu et al.[9]	103
$MoSe_2$	Gu et al.[9]	54
$MoTe_2$	Zhang et al.[10]	~79
WS_2	Han et al.[11]	262.78
WSe_2	Gu et al.[9]	53
WTe_2	Zhang et al.[10]	~40
SnSe	Sun et al.[12]	5.58 (*b* direction) 5.01 (*c* direction)
SiSb	Huang et al.[13]	4.75
GeSb	Huang et al.[13]	7.89
SnSb	Huang et al.[13]	18.21
InS	Shafique et al.[14]	57.1
InSe	Shafique et al.[14]	44.4
InTe	Shafique et al.[14]	33.1
SnP_3	Wei et al.[15]	3.1

2. The electronic band structure of graphether employing the PBE and HSE06 hybrid functionals

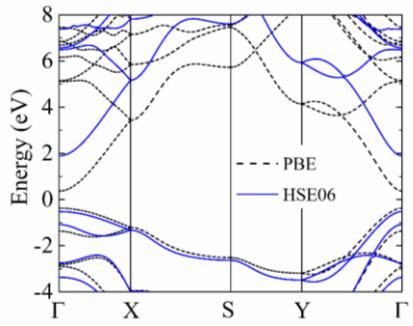

Figure S1. The electronic band structure of graphether. The black dashed and the blue solid lines indicate calculation results employing the PBE and HSE06 hybrid functionals, respectively.

3. The cohesive energies of some 2D doped graphene structures

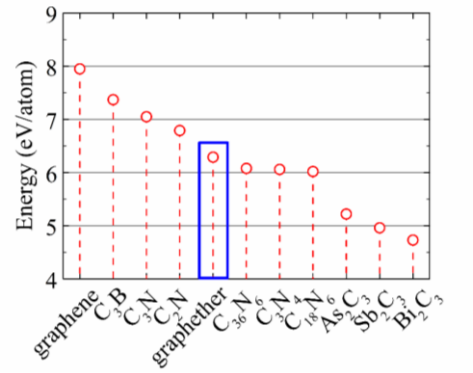

Figure S2. The cohesive energies (eV/atom) of graphether, graphene, C_2N, C_3N, C_3B, C_3N_4, $C_{36}N_6$, $C_{18}N_6$, As_2C_3, Sb_2C_3, and Bi_2C_3. The calculated cohesive energies (eV/atom) of graphether, graphene, C_2N, C_3N, C_3B, C_3N_4, As_2C_3, Sb_2C_3, and Bi_2C_3 are calculated by ourselves, which are similar to other DFT work (graphene: 7.91 eV/atom,[16] As_2C_3: 5.16 eV/atom,[17] Sb_2C_3: 4.89 eV/atom,[17] and Bi_2C_3: 4.66 eV/atom[17]). The results of $C_{36}N_6$ and $C_{18}N_6$ are obtained from other DFT work.[18]

4. The total energies of some 2D doped graphene structures

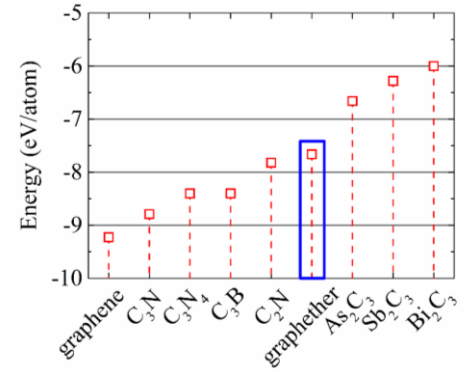

Figure S3. The calculated total energies (eV/atom) of graphether, graphene, C_2N, C_3N, C_3B, C_3N_4, As_2C_3, Sb_2C_3, and Bi_2C_3. All the results are calculated by ourselves, which are similar to other DFT work (graphene: -9.23 eV/atom,[19] C_3N: -8.80 eV/atom,[19] and C_3N_4: -8.37 eV/atom[20]).

5. The cumulative lattice thermal conductivities as a function of phonon mean free paths of graphether and graphene

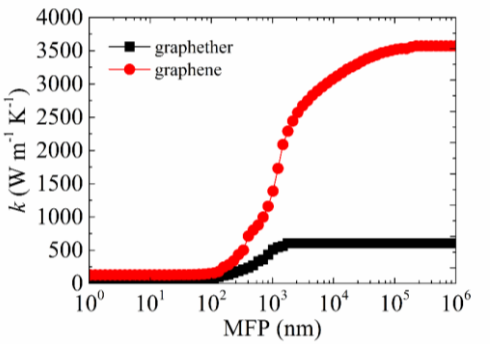

Figure S4. The cumulative lattice thermal conductivities with respect to phonon mean free paths of graphether and graphene at 300 K.

References

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