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Supporting Information

Negative Gaussian Curvature Induces Significant Suppression of Thermal Conduction in Carbon Crystals

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The definition and calculation of Gaussian curvature

The Gaussian curvature *K* at a given surface point is given by the dot product of two principal curvatures ($\boldsymbol{k}_1$ and $\boldsymbol{k}_2$) as[1, 2]

$$K = k_1 \cdot k_2 , \quad \text{(S1)}$$

$$k_1 = \frac{1}{r_1}, k_2 = \frac{1}{r_2}, \quad \text{(S2)}$$

where r_1 and r_2 are the curvature radius with vectors along different principal curvatures, respectively (see Fig. S1). By measuring the curvature radius, the Gaussian curvature value for each carbon allotrope can be calculated based on Eq. S1 and S2.

In order to have a positive Gaussian curvature value, both r_1 and r_2 (i.e., k_1 and k_2) should have the same sign (i.e., both positive or both negative), such as the case of the fullerene C_{60}. For *K* to be zero, either $r_1 = \infty$ or $r_2 = \infty$, such as the case of CNT ($\boldsymbol{k}_1 \neq 0$, $\boldsymbol{k}_2 = 0$), or both $r_1, r_2 = \infty$, such as the case of graphene ($\boldsymbol{k}_1 = \boldsymbol{k}_2 = 0$). Therefore, both CNT and graphene belong to the zero Gaussian curvature structures. For *K* to be a negative number, such as NCCCs in this work, the r_1 and r_2 must have *opposite* signs, i.e., curving in the *opposite* directions (See Fig. S1).

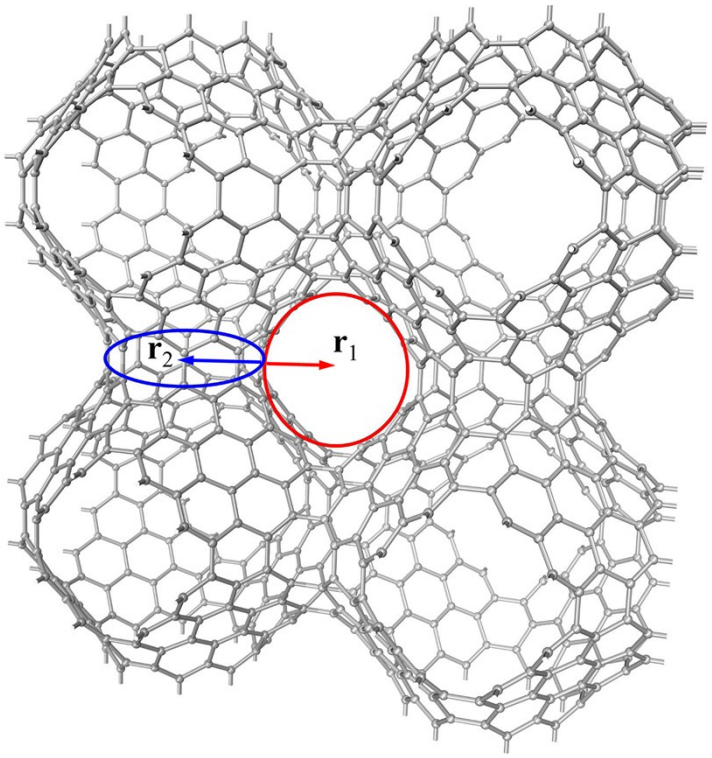

Figure S1| The schematic figure for the calculation of Gaussian curvature in NCCCs.

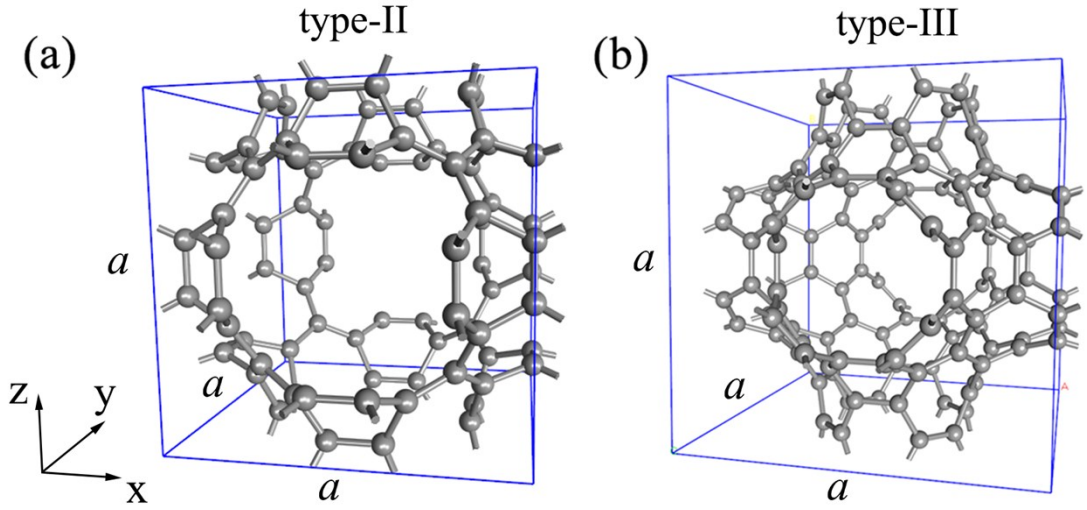

Figure S2| The side view of type-II (a) and type-III (b) unit cell of NCCCs. Here, the variable *a* denotes the lattice constant for each structure.

TABLE SI| Type-II or type-III NCCCs, space group, lattice constant, number of atoms in the cubic cell and fractional coordinates are given.

Name	SPGR	Lattice constant (Å)	N atom	x	y	z
type-II	PM$\bar{3}$M (211)	8.763	80	0.34147	0.14419	0.14419
				0.18779	0.41663	0.00000
				0.21262	0.21262	0.21262

Name	SPGR	Lattice constant (Å)	N atom	x	y	z
III-Type	PM$\bar{3}$M (211)	11.261	128	0.43502	0.25754	0.11054
				0.38123	0.29405	0.00000
				0.21461	0.21461	0.37117
				0.26634	0.26634	0.26634

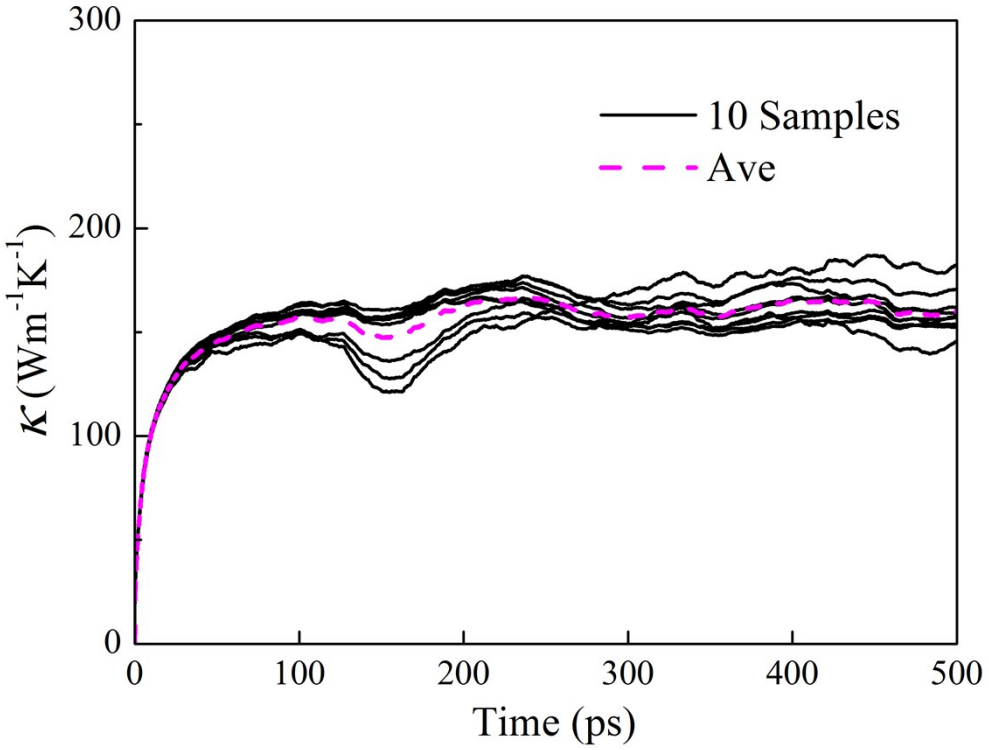

Figure S3| Time convergence in Green-Kubo simulations of thermal conductivity.

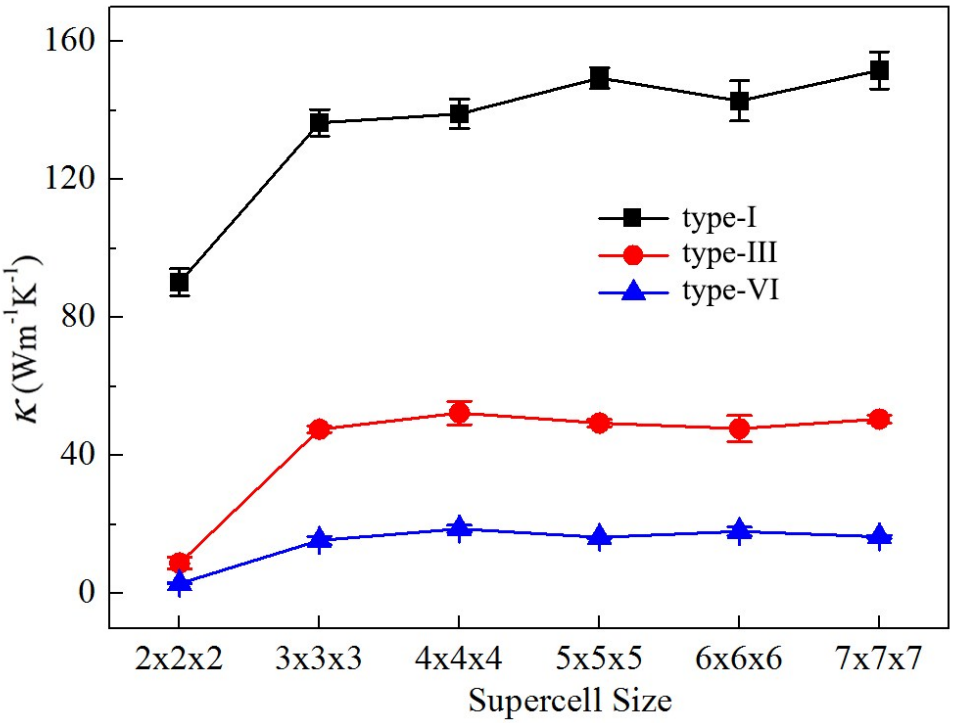

Figure S4| Size convergence in Green-Kubo simulations of thermal conductivity.

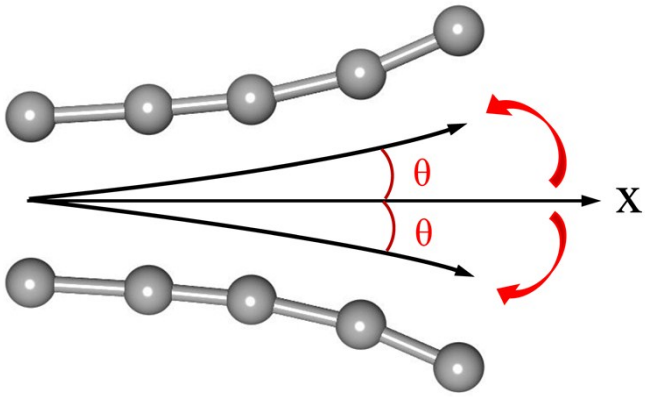

Figure S5| Schematic figure of surface curving with angle θ away from x direction.

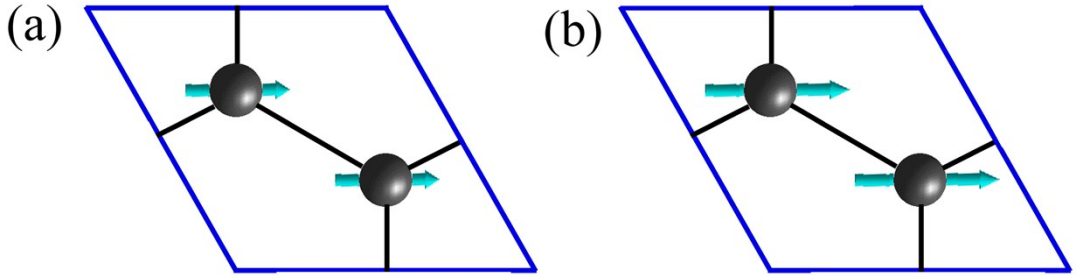

Figure S6. Vibration displacement of TA mode in graphene at Γ point (a) and half of the *k*-point along [100] direction (b), respectively.

References

1. S. Gupta and A. Saxena, *J. Appl. Phys.*, 2011, **109**, 074316.
2. S. Gupta and A. Saxena, *J. Appl. Phys.*, 2012, **112**, 114316.