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Low lattice thermal conductivity of a 5-8-peanut-shaped carbon nanotube

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1. Verification of Tersoff potential

We calculate the C-C bond lengths in 5-8-PSNT with the Tersoff potential using molecular dynamics (MD) simulation and compare them with the results of density functional theory (DFT) calculation to verify the accuracy of the Tersoff potential. As shown in **Fig. S1**, the C_1-C_2, C_2-C_3 and C_3-C_4 bonds in the connection part and C_5-C_6, C_5-C_7 and C_7-C_8 bonds in the cage are close to each other, respectively, in the two optimized structures, showing that the Tersoff potential we choose is appropriate to describe the carbon-carbon interactions in the 5-8-PSNT structure.

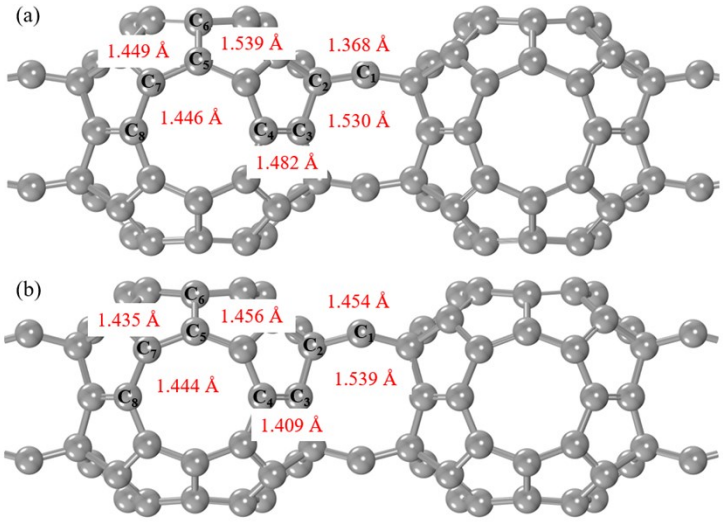

Fig. S1 Optimized structure of 5-8-PSNT by using (a) MD and (b) DFT calculations.

2. Thermal conductivities with error bars

We calculate the error bars for 5-8-PSNT and (6,6) CNT. Because the thermal conductivities of 5-8-PSNT are much smaller than those of (6,6) CNT, to clearly show the error bars, we plot the results separately, as shown in Fig. S2 (a,b).

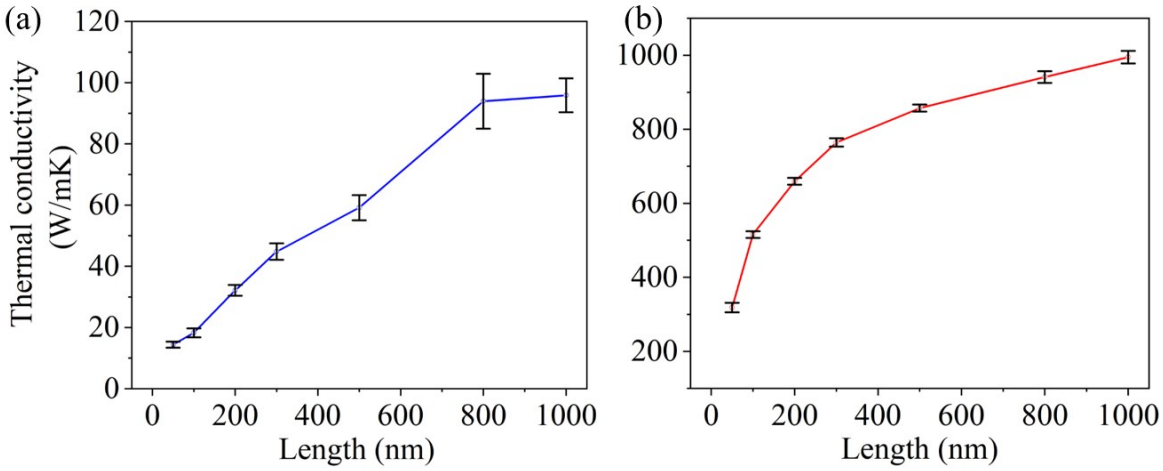

Fig. S2 Variation of the thermal conductivity with the length with error bars for (a) 5-8-PSNT and (b) (6,6) CNT.

3. Temperature-dependence of the thermal conductivity

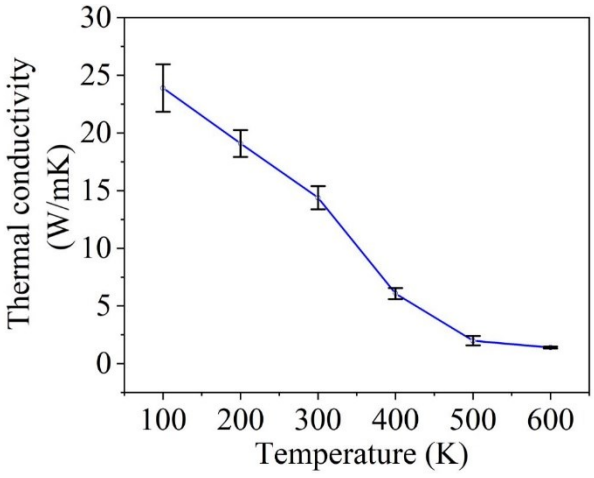

Fig. S3 Variation of the thermal conductivity with temperature for 5-8-PSNT.