Supplementary Materials

A C_{20} fullerene-based sheet with ultrahigh thermal conductivity

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1. Isotopic scattering rates and three-phonon scattering

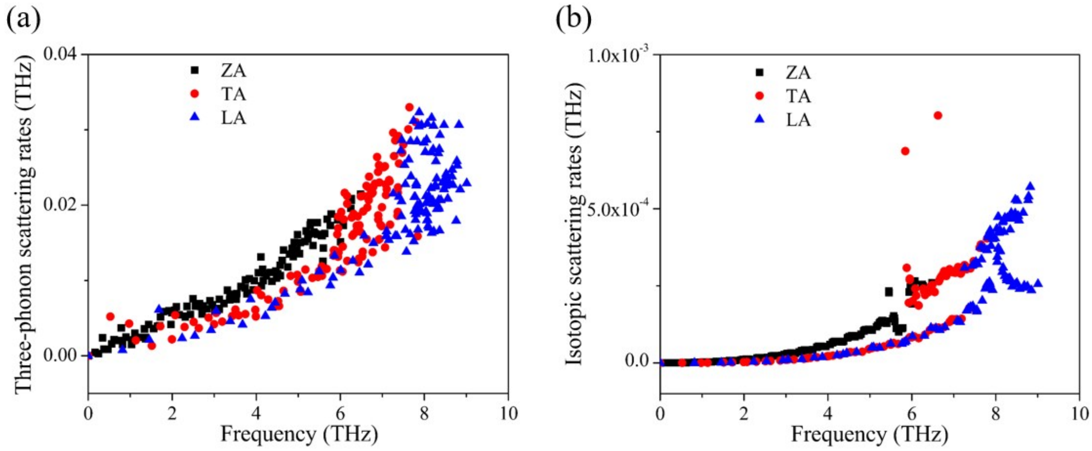

Fig. S1 Variation of (a) the isotopic scattering rates, and (b) the three-phonon scattering rates of the acoustic branches with frequency at 300 K for Hexa-C_{20}

2. Elastic constants of Hexa-C_{20}

Table S1. Calculated elastic constants (units of Nm^{-1}) of Hexa-C_{20}

C_{11}	522.5
C_{12}	36.9
C_{13}	4.6
C_{22}	522.5
C_{33}	15.4
C_{44}	242.5

3. Possible way to synthesize Hexa-C_{20}

A possible way to synthesize Hexa-C_{20} is using laser ablation of polycrystalline diamond or graphite on some proper substrates. The possibility has been demonstrated by the synthesis of a C_{20}-based solid,[1] where the solid phase of dodecahedral C_{20} can be acquired on the nickel substrates in the presence of 10^{-4} torr of cyclohexane or benzene with the pulsed laser ablation at a wavelength of 248 nm on the polycrystalline diamond.

4. Structural information of the optimized Hexa-C_{20}

Lattice parameters: a = b = 6.9639Å, c = 15.4007Å.

Space group: P6/mmm (191)

Atomic Wyckoff positions:

Table S2. Atomic Wyckoff positions of Hexa-C_{20}

Wyckoff positions	x	y	z
12o	-0.21117	0.57766	0.41847
6m	-0.12987	0.74026	0.50000
4h	0.33333	0.66667	0.45055
12n	0.40210	0.00000	0.38233

References

1 Z. Iqbal, Y. Zhang, H. Grebel, S. Vijayalakshmi, A. Lahamer, G. Benedek, M. Bernasconi, J. Cariboni, I. Spagnolatti and R. Sharma, *Eur. Phys. J. B.*, 2003, **31**, 509-515.