Supporting Information for

Tunable thermal transport and mechanical properties of graphyne heterojunctions

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1. Model of GY sheets

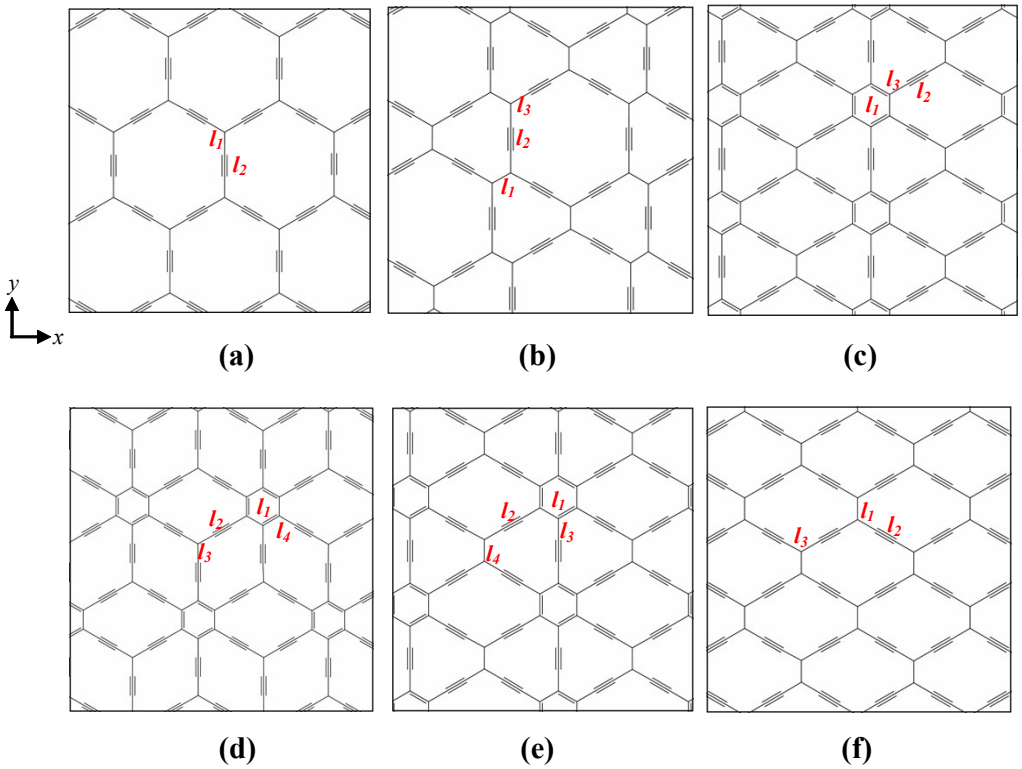

Figure S1 . The geometric structures of the 2D graphyne allotropes: (a) α-, (b) β-, (c) γ-, (d) δ-, (e) 6,6,12- and (f) 14-graphyne sheets. l_1, l_2, l_3 *and* l_4 are the bond length. The *x* and *y* axis along the zigzag and armchair directions, respectively.

2. Thermal conductivity of GY sheets

The structures of δ-GY is shown in Fig. S2(a). The outmost atoms highlighted with blue are defined as "cold slab", and the middle atoms highlighted with red are defined as "hot slab". Fig. S2(b) shows the temperature profile of δ-GY. The temperature profile is symmetrical, while the nonlinear temperature profile occur near cold and hot regions. The linear portion (solid red line in Fig. S2b) is selected to calculate the temperature gradient. The thermal conductivity for γ-GY with 20 nm × 20 nm is 18.7 W/mk in the armchair direction and 18.6 W/mk in the zigzag direction, which are consistent with the previous MD results[1] using Airebo potential (17.66

W/mk in both armchair and zigzag directions). Fig. S2(c-d) shows the curve of inverse of thermal conductivity versus the inverse of length.

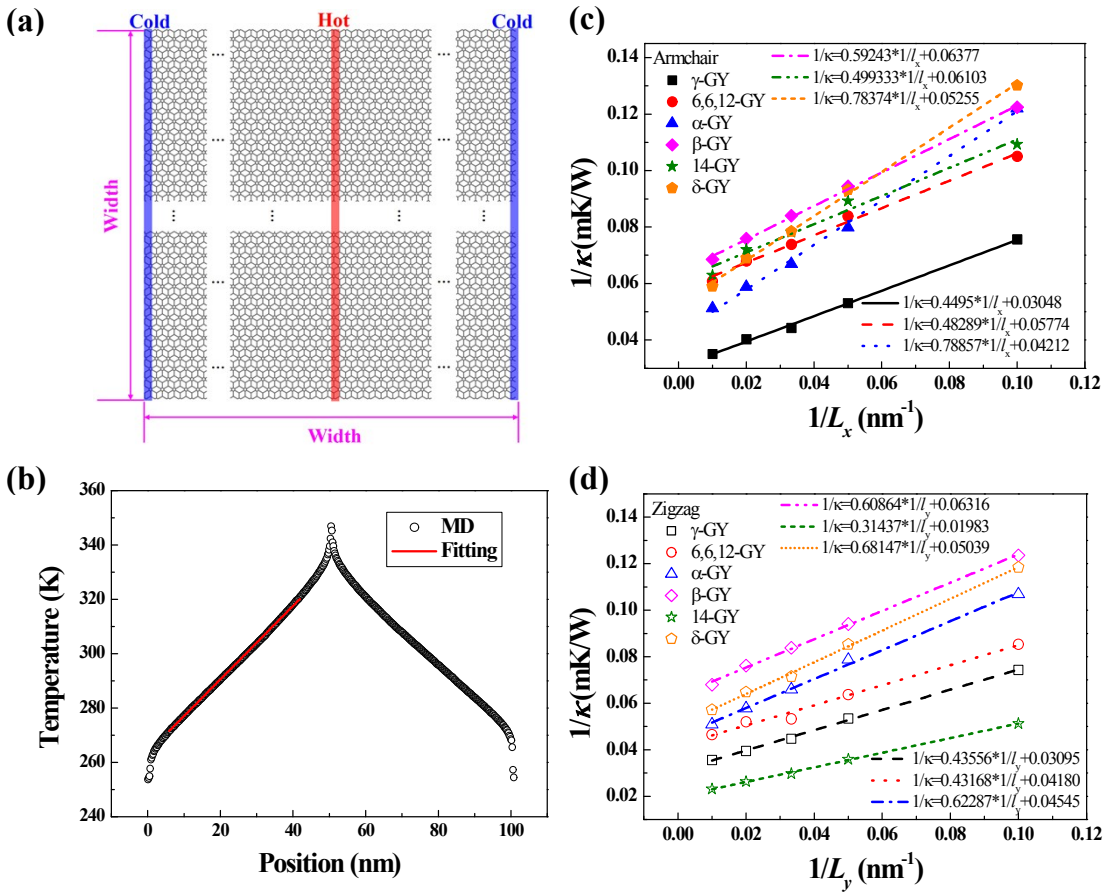

Figure S2. (a) Schematic diagram of the NEMD model for δ-graphyne at the temperature T = 300 K. The atoms highlighted with blue and red represent the cold and hot regions, respectively. (b) The corresponding temperature profile (the red line indicated the temperature gradient). The inverse of thermal conductivity ($1/\kappa$) versus the inverse of length ($1/l_b$) for six graphynes in the armchair (c) and zigzag direction (d). l_x and l_y indicated the heat flux direction along the x and y axis, respectively.

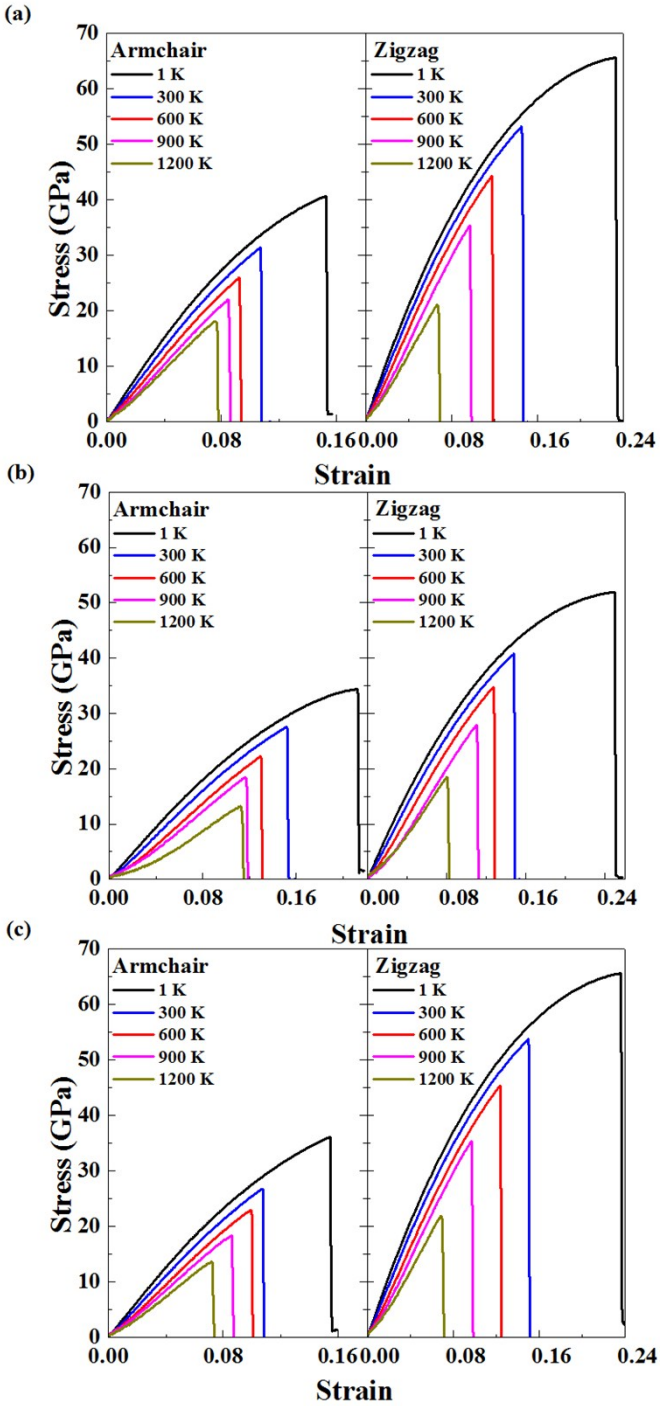

Figure S3. Stress-strain curves of (a) γ-GY/14-GY/γ-GY, (b) α-GY/14-GY/α-GY and (c) 6,6,12-GY/14-GY/6,6,12-GY sheets with uniaxial tension along the armchair and zigzag directions at various temperatures from 1 K to 1200 K. The percentage of each graphyne in the GYHJ is approximately 50%.

References

1. Y. Zhang, Q. Pei and C. Wang, *Comp. Mater. Sci.*, 2012, **65**, 406-410.