Supplementary information for

Mechanical and thermal properties of graphyne-coated carbon nanotubes: A molecular dynamics simulation on one-dimensional all-carbon van der Waals heterostructures

1. Supplementary table

Tab. S1 The thermal conductivity of CNT and GNT with different chiralities

	Armchair-CNT	Zigzag-CNT	Armchair-GNT	Zigzag-GNT
k (W/mK)	156.79	149.26	9.81	10.01

2. The details of the AA, AZ, ZA and ZZ structures of CNT@GNT

Unless otherwise specified, in the present study the AA structure represents (15,15)CNT@(7,7)GNT, AZ structure represents (15,15)CNT@(12,0)GNT, ZA structure represents (26,0)CNT@(7,7)GNT and ZZ structure represents (26,0)CNT@(12,0)GNT, respectively. In addition, the length of CNT@GNT is determined by the number of its unit cell in the axial direction. A CNT@GNT unit cell requires a pairing with the smallest value of the percentage of length mismatch of its CNT and GNT components. The numbers of CNT and GNT unit cells used to construct a CNT@GNT unit cell are listed in Tab. S2.

Tab. S2 Numbers of CNT and GNT unit cells in a unit cell of CNT@GNT with different chiralities

	Number of CNT unit cells	Number of GNT unit cells
AA	82	29
AZ	78	16
ZA	46	28
ZZ	45	16

3. Supplementary figure

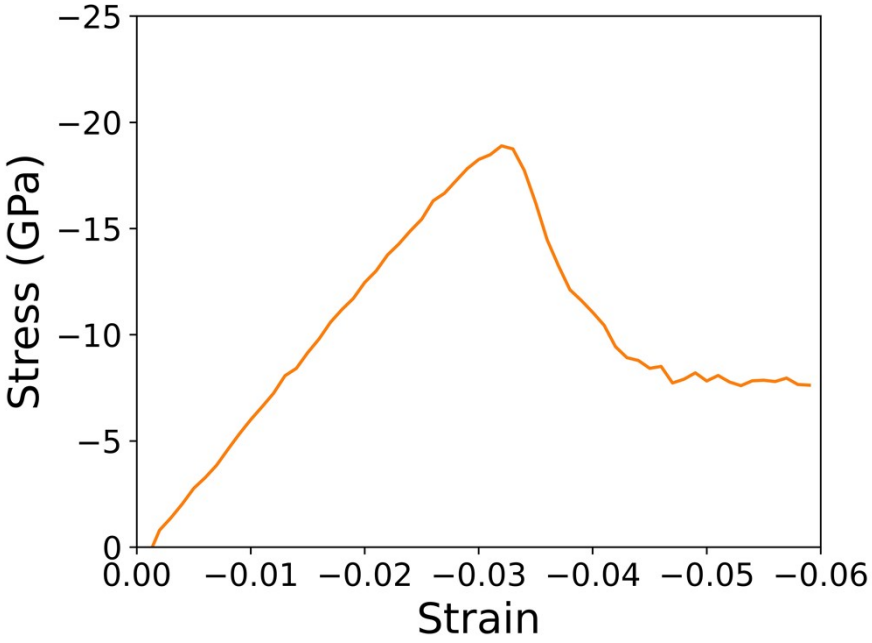

Fig. S1. Stress-strain curves for CNT@GNT under compression.