

# **Size- and Chirality-Dependent Mechanical Properties of Single-Walled Phenine Nanotubes**

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## **Supporting Materials**

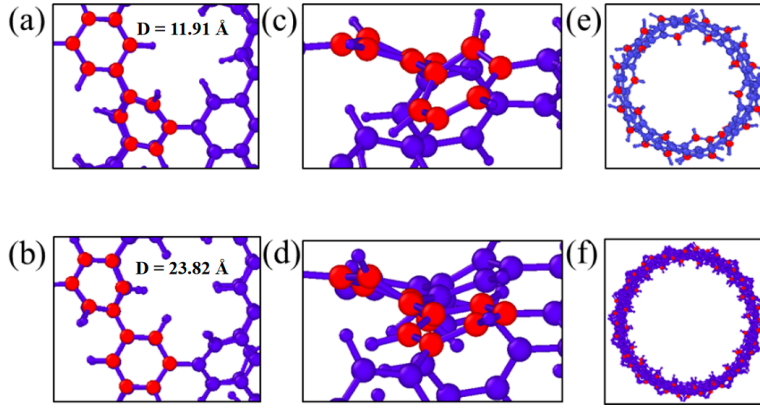


Figure S1. Twisting behavior of linear carbon chains in PNTs. a and b, local structures of twisted benzene rings during relaxation, c and d, side view of the adjacent benzene ring after twisting, e and f, cross-section of the corresponding PNTs. The atoms marked in red are carbon atoms in the benzene ring structure that undergo torsion.

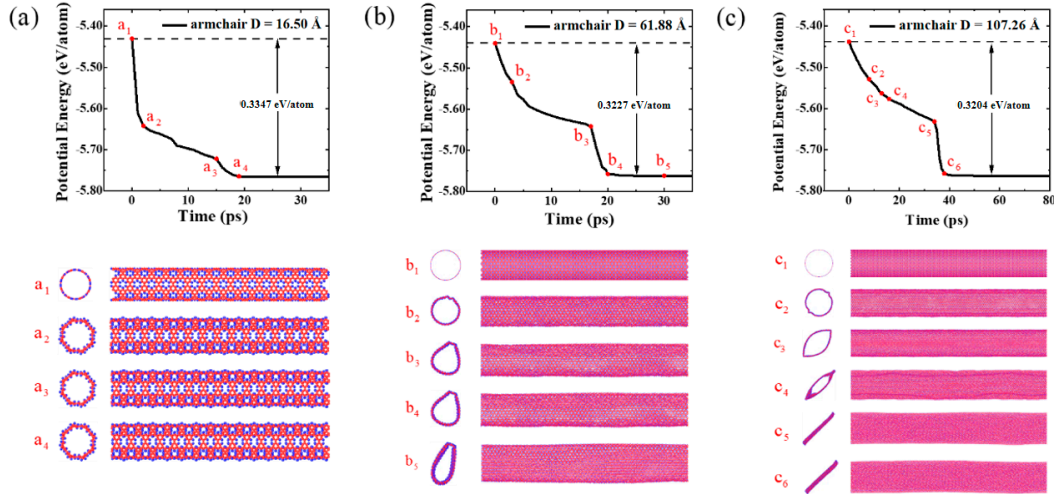


Figure S2. Structural evolution for 3 selected armchair PNTs as a function of time, the corresponding potential energy are plotted in the top panel, while the snapshots are shown in the bottom.

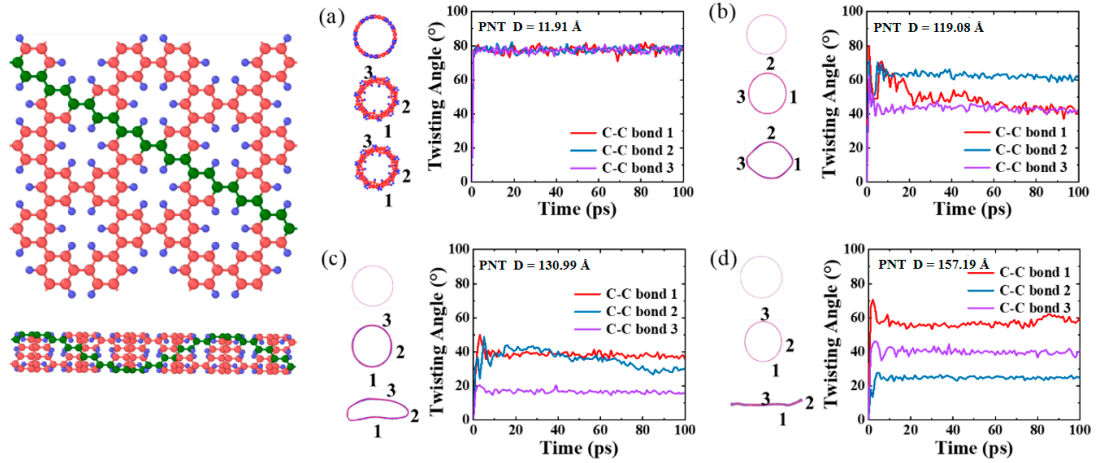


Figure S3. Twisting of helical carbon chains in zigzag PNTs. (a-d) present selected twisting angle evolution as a function of time for PNTs with different diameters.

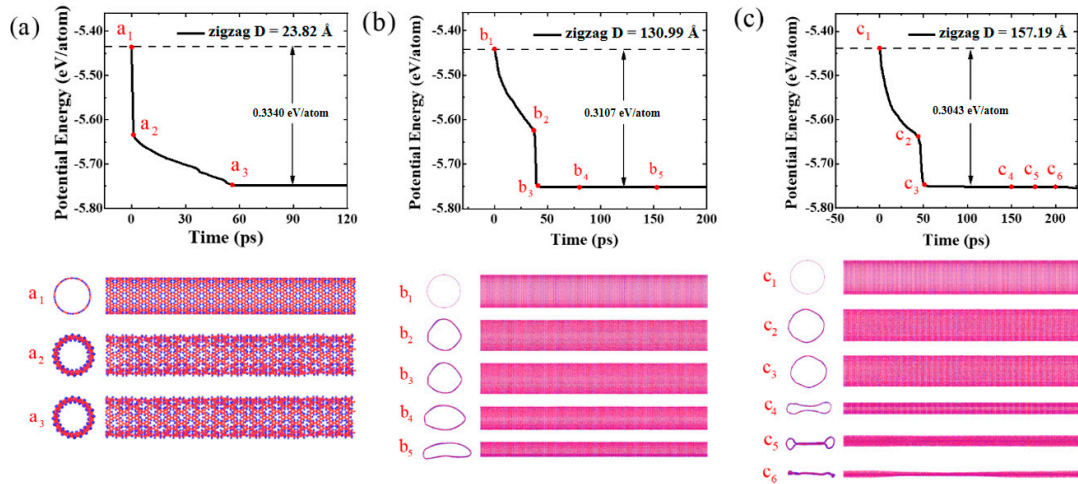


Figure S4. Structural evolution for 3 selected zigzag PNTs as a function of time, the corresponding potential energy are plotted in the top panel, while the snapshots are shown in the bottom.

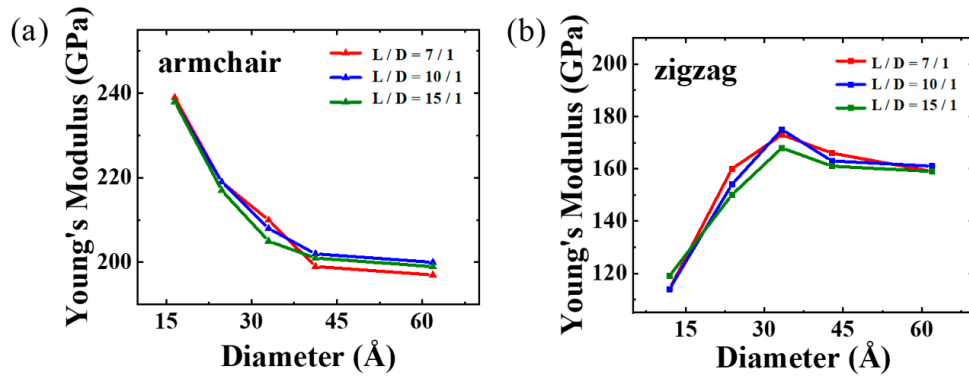


Figure S5, Young's modulus of PNTs under tensile loadings.

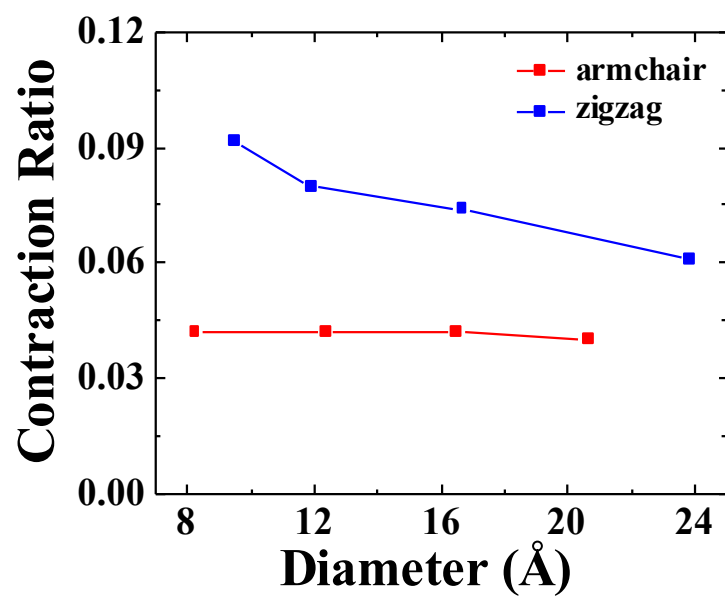


Figure S6, Contract of PNT length when rolled up from defected graphene sheets.