Edge-reconstructed, Few-layered Graphene Nanoribbons: Stability and Electronic Properties

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Supplementary Information

New carbon structures from reconstructed few-layer graphene edge

We have performed first-principles calculations for the graphene/nanotube hybrid system reported in Ref. 5 under tensile strain. The system, as shown in Fig. 1, consists of a $(10, 0)$ carbon nanotube hybridized, through sp^3 bonds, to a five-layer graphene sheet. Tensile strain is applied parallel to the graphene basal plane and perpendicular to the nanotube axis. The left panel of Fig. 1 shows the corresponding stress-strain curve for such strain direction. Particular points in this curve are marked for 10% to 13% strain values, and the corresponding structures of the hybrid system at those strain values are shown in the right panel. The figure shows that, for a strain of 13%, a complete rupture of the hybrid system occurs, with the detachment of the nanotube and the rupture of the five-layer graphene sheet. After further geometry optimization, the border of the ruptured five-layer graphene sheet assumes the geometry of the reconstructed five-layer graphene edge of Fig. 1(c) (see main text).

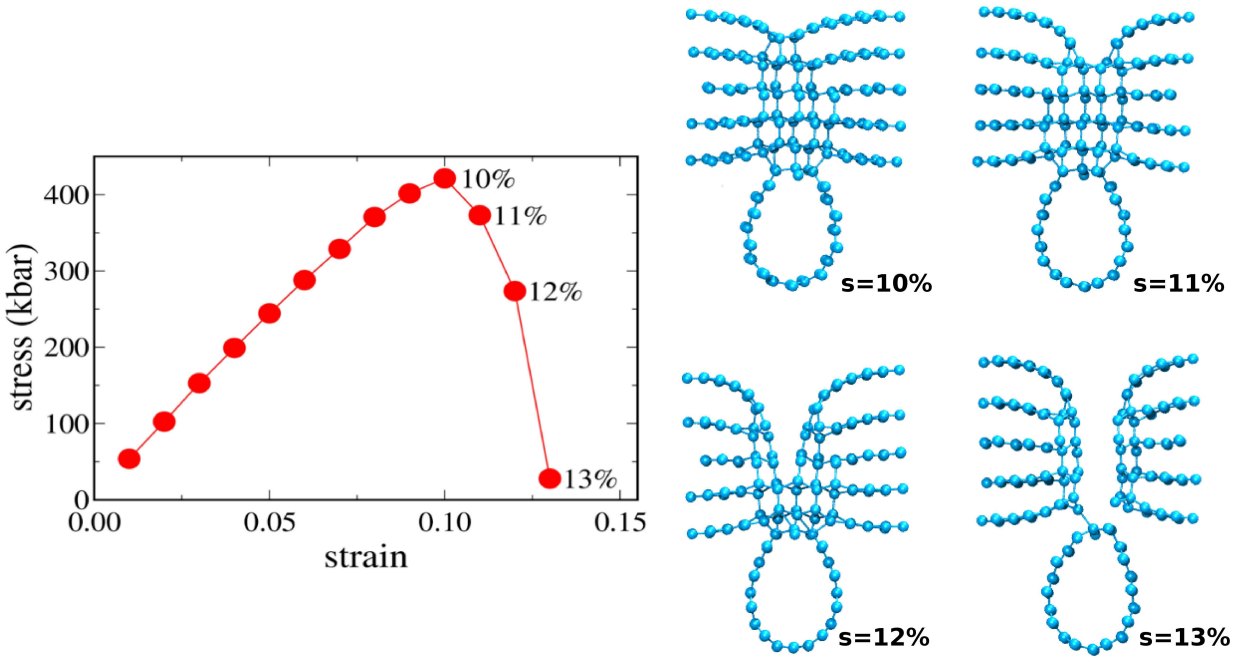

Figure 1: Hybrid system formed by five graphene layers and one $(10, 0)$ carbon nanotube under tensile strain applied parallel to the graphene basal plane. On the left, the corresponding stress-strain curve. On the right, final structure for the selected strain values, respectively; 10%, 11%, 12% and 13%, where it is possible to see the rupture of the system.