Mechanics of rolling of nanoribbon on tube and sphere

(Supplementary Information)

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To verify if the torsional energy of GNR has contribution to the total energy, we performed MD simulation with a GNR winding onto a tube in helix form. The GNR with 87.048 angstrom in length and 12.564 angstrom in width is chosen to interact with an infinitely long CNT with a radius of 5.388 angstrom (SFig. 1). We marked α as the angle between helical direction and the axis of the CNT and h as the distance of the two farthest ends of the GNR. Changing h would lead to the change of the torsional energy. SFig. 1 shows the relationship of the potential energy per atom of the ribbon against h. The difference between the maximum and the minimum is 0.0015 eV per atom which is 0.02% of the potential energy (~6.95 eV per atom). So we ignored the influence of torsional energy in our model.
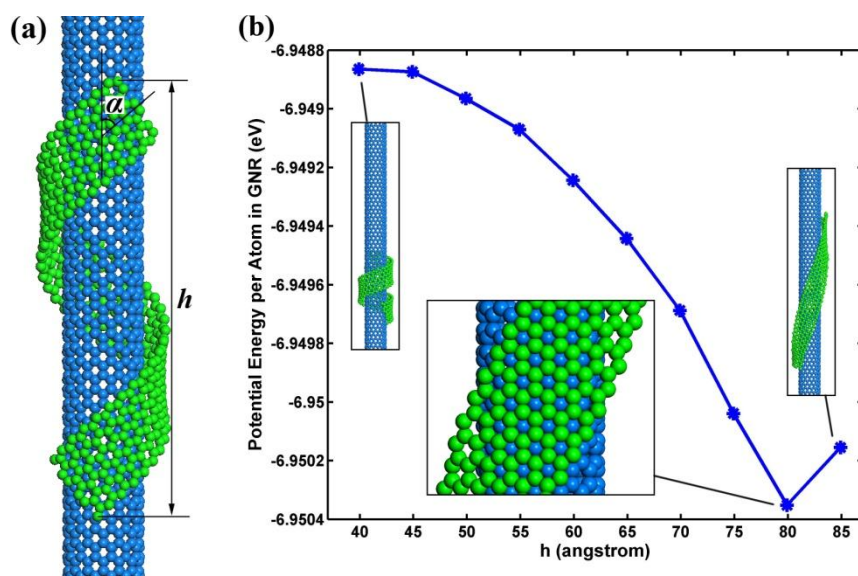
SFig. 1 The relationship of the total potential energy of GNR with the parameter h.