Mechanics of rolling of nanoribbon on tube and sphere

(Supplementary Information)

Qifang Yin, Xinghua Shi*

LNM, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190

*shixh@imech.ac.cn

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 $\alpha$ 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 $h$. 