

# Reconstruction and Evaporation of Edge Carbon Atoms of Graphene Nanoribbons

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The reconstruction and evaporation of carbon atoms at edge of graphene nanoribbons are investigated by performing tight-binding molecular dynamics simulation and ab initio calculation. In this study, it is observed that the zigzag edge is very quickly reconstructed into the zigzag pentagon-heptagon edge which is found to be more favorable by ab initio total energy calculation and the reconstruction helps carbon atoms to evaporate easily. Commonly in the zigzag and armchair edge, the evaporation of carbon atoms is preceded by the formation of heptagon rings which work as exits of carbon atoms into vacuum. In the tight-binding molecular dynamics simulation of armchair graphene nanoribbon, the formation of zigzag edge accelerates the evaporation of carbon atoms and finally the continuous evaporation draws the formation of carbon linear chain between the patches of zigzag edge, which are in excellent agreement with recent transmission electron microscopy[1,2]. In the tight-binding molecular dynamics simulation for graphene nanoribbon junction of armchair-zigzag-armchair, carbon atoms are evaporated in row after row from the outermost row of zigzag edge while the armchair edge almost keeps the structure.

[1] S. Iijima et al Phys. Rev. Lett. 102, 205501 (2009)

[2] A. Zettl et al. Science 323, 1705 (2009)