Reconstruction of Vacancy Defects in Graphene and Carbon Nanotube

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Various structures of vacancy defects in graphene layers and carbon nanotubes have been reported by high resolution transmission electron microscope (HR-TEM) and those arouse an interest of reconstruction processes of vacancy defects. In this talk, we present reconstruction processes of vacancy defects in a graphene and a carbon nanotube by tight-binding molecular dynamics (TBMD) simulations and by first principles total energy calculations. We found that a structure of a dislocation defect with two pentagon-heptagon (5-7) pairs in graphene becomes more stable than other structures when the number of vacancy units is ten and over. The simulation study of scanning tunneling microscopy reveals that the pentagon-heptagon pair defects perturb the wavefunction of electrons near Fermi level to produce the $\sqrt{3} \times \sqrt{3}$ superlattice pattern, which is in excellent agreement with experiment. It is also observed in our tight-binding molecular dynamics simulation that 5-7 pair defects play a very important role in vacancy reconstruction in a graphene layer and carbon nanotubes.