Graphene Growth and Electronic Structure of Graphene and Graphene-based Nanostructures

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Recently, interesting subjects in graphene research is the growth mechanism of single layer graphene sheet on various substrates and the band gap engineering of pristine gapless graphene. First, we have performed density functional theory (DFT) calculations to understand the initial stage of graphene growth by investigating adsorption behaviors of carbon atoms on the oxide substrates such as sapphire and magnesium oxide. The single carbon atom is found to bind favorably to an oxygen atom on the surface. By increasing the number of adsorbed carbon atoms, we study binding behaviors of carbon atoms on the oxide surfaces. Noticeably, at least one carbon atom of the carbon structure binds to an oxygen atom of the surfaces due to relatively strong bond between carbon and oxygen atoms. Combined with the experimental results, these theoretical findings may imply that carbon atoms on the oxide substrates form the nanocrystalline graphite structure rather than a perfect graphene, within a limited area. On the other hand, in relation to the limitation of gapless graphene, many interesting studies have been focused on its functionalization such as oxygen adsorption and also on functionalization of graphene-based nanostructures. The periodically modulated graphene (PMG) generated by nano-patterned surfaces is reported to profoundly modify the intrinsic electronic properties of graphene. DFT calculations performed on a model of PMG reveals a possible tuning of a band gap by considering both strain caused by periodic bending of graphene and doping through chemical interactions with underlying substrate oxygen atoms. Also, we have studied the edge-functionalization of armchair graphene nanoribbons (AGNRs) with pentagonal-hexagonal edge structures. Electronic structures of these edge-functionalized AGNRs vary depending on the number of electrons, supplied by substitutional atoms, at the edges.