Theoretical Study on Strain Relaxation of Graphene by Functionalization Reaction

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Covalent functionalization is one of the methods to modify electronic structures of graphene to change graphene to a semiconducting material. It has been reported that strain affects the reactivity of graphene functionalization. To elucidate the relationship between strain and functionalization reaction, density functional theory (DFT) calculation was conducted considering functional groups and their coverages; hydrogen and phenyl groups with different coverages. Binding energy of functional groups and graphene deformation energy were calculated to interpret the stability of functionalized graphene. The bond length of graphene was also analyzed to explain the change of strain by functionalization. Interestingly, we found that the graphene was extended in high coverage but compressed in low coverage. In addition, we investigated the physical and electronic interactions between Cu substrate and graphene and compared strain effects to pure graphene system. Overall, we elucidated strain change of graphene by functionalization reaction related with functional groups, their coverages and Cu substrate effect.