Theoretical Study on Peculiar Relationship between Graphene Strain State and Functionalization

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Graphene as semiconducting material requires electronic structure modification, which can be easily achieved through graphene functionalization. To facilitate the functionalization reaction, mechanical strain on graphene was applied. Experimentally, strain relaxation after functionalization reaction has been reported with 2D Raman spectra results. Thus, density functional theory (DFT) calculation was conducted to understand the correlation between strain and functionalization behavior by considering functional groups and their coverage effects. Binding energy of functional groups and structural deformation energy of graphene were calculated to elucidate how the strain changes in the functionalized graphene. Interestingly, under high coverage of functional groups, expansion of graphene was observed, while compression was observed with low coverage of functional groups. Cu substrate effect was also investigated to understand electronic structure changes in the presence of substrate. In conclusion, we uncovered the correlation between strain state and functionalization of graphene, considering both its coverage and Cu substrate effect.