Theoretical Study on Strain Relaxation of Graphene by Functionalization Reaction

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Graphene formed on the Cu substrate through chemical vapor deposition (CVD) is compressed due to thermal coefficient mismatch. It has been reported that the compressive strain of graphene is released when the functionalization occurs. For fundamental understanding of strain relaxation by graphene functionalization, density functional theory calculation was conducted. Total energies of graphene under different compressive strain (~1%) were relatively compared. Binding energy of phenyl group and deformation energy of graphene were calculated to obtain the total energy change of functionalized graphene. The effect of functionalization density was also investigated with various functionalization coverage. Interestingly, we found that functionalization released the strained graphene at high functionalization density but compressed the graphene at low functionalization density. Additionally, the mechanical and electronic interaction between Cu substrate and graphene were investigated.