Structural and electronic properties of hydrogenated sp^3 multilayer graphene

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We studied how multilayer graphene can undergo transformation into sp^3 bonded structure using the density functional theory calculation. Hydrogenation of multilayer graphene at top and bottom layer induces sp^2 to sp^3 transition. Hydrogenated surface reduces the transition barrier of sp^3 multilayer graphene due to low stability of hydrogen passivated graphene layer caused by unpaired electron. The transformation occurred depending on the number of graphene layers and hydrogen coverage. As number of layer is lower and hydrogen coverage is higher, the transformation into sp^3 multilayer graphene becomes easier. Electronic and mechanical properties of sp^3 multilayer graphene were also obtained by varying the number of layers and stacking structure of sp^3 multilayer graphene. We found that sp^3 bonded structure induced from multilayer graphene can have tunable band gap and Young's modulus, which reveals their potential usage for the electronic devices.