Prediction of sp^3-tized diamond like structure induced by surface hydrogenation of multilayer graphene

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We investigated multilayer graphene transformation into sp^3 structure using density functional theory (DFT) calculation and predicted diamond-like properties in multilayered sp^3 structures at various thickness. The hydrogen atom adsorptions onto both surface sides of the multilayer graphene induced the transformation of the multilayer graphene into the sp^3-hybridized structure with small energy barrier and large heat of reaction. As the number of sp^2 layer decreased and hydrogen adsorption became relatively large, the transformation of the sp^2 structure into sp^3 configured structure became energetically favorable. Further, electronic and mechanical properties of sp^3 multilayer graphene were calculated by varying the number of layers and the stacking order of the sp3 structure. The sp^3 structure exhibited various band gap (2.2~3.5 eV) and Young's modulus (700 ~ 1050 GPa) indicative of a diamond material, except that the electrons of conduction band were mainly located at the hydrogenated surface. By extrapolating the band gap, Young's modulus and structure properties, we theoretically predicted that the thinnest possible sp3 structure, that could contain diamond-like properties.