Theoretical study on graphene hydrogenation via Birch reduction : Chair vs Boat-type configuration

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In this theoretical study, we elucidated overall reaction scheme of graphene hydrogenation using Birch-type reaction by predicting energetically favorable configurations of Li, NH_3 and t-BuOH on copper substrate. Li played a crucial role for the graphene hydrogenation; in addition to reducing graphene, Li^+ ion weakened the binding energy between H and O atoms in OH group. More importantly, Li^+ ion made the reaction thermodynamically and kinetically favorable by reducing the heat of reaction (i.e. $3Li^+ \rightarrow$ exothermic reaction) and energy barrier. We found that the boat-type configuration of graphene was more favorably formed on Cu substrate because of less repulsive interaction exerted on H atom in OH group with help of neighborly chemisorbed H atom and Li^+ ion. Also, the formation energy result confirmed that the boat-type was always more favorable due to unpaired electrons of carbon atoms. Thus, based on this thermodynamic analysis, we conjecture that fully hydrogenated graphene of boat-type configuration on Cu substrate can be synthesized through the Birch reduction reaction.