Prediction of Graphene Hydrogenation Assisted by Birch Reduction and Hot Electron

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Hydrogenation of graphene has received much attention for practical electron device applications mainly due to its band gap opening. Although wet chemical reaction such as Birch reduction is a promising method to synthesize the hydrogenated graphene, the low coverage of hydrogenation is still an issue. In this study, through multiscale computational approach, we suggest a potential experimental method to enhance the reactivity of graphene hydrogenation by combining with Birch reduction and hot electron effect. We firstly verified the hot electron transfer from gold nanoparticle to graphene through discrete dipole approximation (DDA) calculation. It showed that the graphene was easily reduced by hot electrons. Next, through density functional theory (DFT) calculation, we confirmed that the reactivity of hydrogenation of graphene by Birch reduction was improved by hot electron. Especially, we predicted that hot electrons can kinetically boost the hydrogenation reaction. Our theoretical study showed that the hydrogenated graphene with high hydrogenation coverage can be experimentally achieved by improving the reactivity of hydrogenation through use of hot electrons.