2P12

Long range functionalization of h-BN monolayer by carbon doping

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The catalytic activation of molecular oxygen is crucial for a number of important industrial chemical processes, such as selective oxidation and epoxidation, exhaust gas emission control for automotive applications, oxygen reduction reaction in fuel cells, and so on. Extensive efforts are devoted to the development of effective catalytic materials for oxygen activation. Currently, most of the industrially used catalysts are based on precious transition metals (Pt, Pd, Ru, etc.). Therefore, the development of effective, cheap and environment friendly catalysts based on the nonprecious abundant elements is a big challenge for commercial market.

Recently, we have demonstrated theoretically and proved experimentally that even inert and catalytically inactive materials can be functionalized; it can become active catalysts at nanoscale by inducing the defects or additional transition metal support [1].

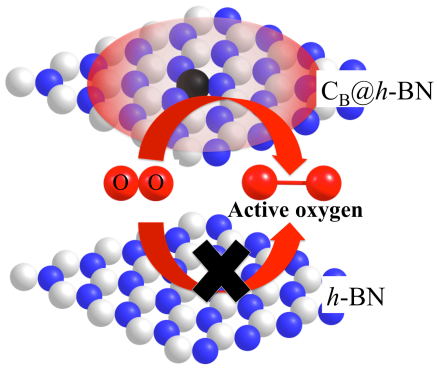

Fig.1 A scheme of the large activation area for O_2 on the C_B@h-BN.

In the present work, we performed a systematic investigation of the catalytic activity of the C doped h-BN monolayer toward a reaction with molecular oxygen reactant. It is demonstrated that C doping into B position on the *h*-BN monolayer (C_B@*h*-BN) produces n-type semiconductor material with noticeable catalytic activity in the large area extended far away from the C impurity (**Fig.1**). The adsorption energy of O_2 on C_B@*h*-BN decreases slowly with the increase in distance from the C impurity, while O_2 remains highly activated. To investigate the catalytic activity of C_B@*h*-BN, the oxygen reduction reaction [2] and oxidation reactions of CO and C_2H_4 are considered. All these reactions can occur even at the sites far from the doped C atom. Such effects were not observed for h-BN monolayer doped with different atoms such as B, N, Al, Si, Ge, Ni, Pt, Pd, and Au where O_2 adsorbs only in the close vicinity of the dopant. Therefore, even small concentration of C dopants can functionalize the large surface area of h-BN monolayer, making it a promising catalytic material.

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[2] Gao M.; Adachi M.; Lyalin A.; Taketsugu T. *J. Phys. Chem. C* **2016**, in press (DOI: 10.1021/acs.jpcc.5b12706)