Theoretical Suggestion and Experimental Proof for Novel Catalyst: Boron Nitride with Gold

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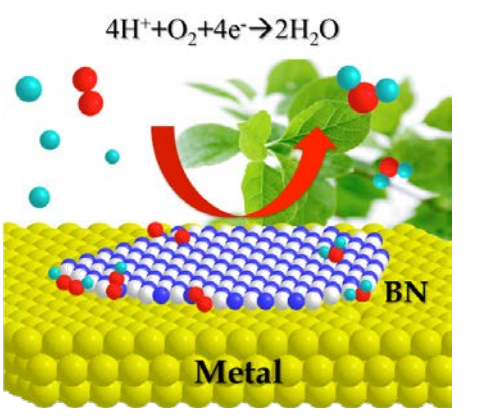
In this talk, we introduce our recent research to design a new catalyst starting from theoretical suggestion. The main idea is that even catalytically inactive or completely inert materials can be functionalized at the nanoscale via the size, structure, morphology, and support effects [1,2]. Oxygen reduction reaction (ORR) is a key process in fuel cells, and the most efficient catalysts for ORR are based on platinum. Since platinum is a noble and rare metal, there are growing a lot of interests to develop alternative catalysts. Recently we theoretically demonstrated that hexagonal boron nitride (h-BN), which is catalytically inert insulator with a wide band gap, can be functionalized and act as an electrocatalyst for ORR. Such functionalization can be achieved by the nitrogen doping or deposition of the BN nanosheets on some transition metals [3,4]. Following theoretical suggestions, catalytic activities of h-BN on Au electrodes were examined experimentally [5]. In this work, however, ORR on the terrace of BN/Au proceeds only via the 2e– mechanism with reduction of OOH* intermediate to H_2O_2, while the 4e– process is not favorable energetically due to stability of OOH* towards dissociation into OH* and O* on BN/Au(111). The stability of OOH* towards dissociation results from the weak adsorption of O* atom on BN/Au(111). Thus, providing sites for stabilization of oxygen would promote the effective 4e– pathway of ORR with formation of H2O. Then, we demonstrated theoretically that gold nanoparticles (Au-NP) supported on BN/Au can provide such active sites for oxygen adsorption, and it was experimentally shown that OOH* dissociation is promoted at the perimeter interface between the Au-NP and BN/Au surface opening the 4e– pathway for ORR [6]. It was also demonstrated that BN/Au can be utilized as catalysts for hydrogen evolution reaction [7].



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