Unveiling Electrochemical Oxygen Reduction Activity of Defective Graphene Basal Plane

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Metal-free carbon nanomaterials have been suggested as one of the potential alternatives to replace Pt-based oxygen reduction electrocatalysts due to their abundance of element resources, facile synthetic approach, and CO tolerance. However, pristine carbon framework (i.e., graphene or carbon nanotubes) is inert for oxygen reduction reaction (ORR) so that their chemical modification is needed to activate carbons. Recently, it was reported that defective carbon edges in heteroatom-free carbon nanomaterial can be used as ORR active sites, while the basal plane is inactive to ORR. Since the basal plane has largely exposed area than edges, the number of potential active sites is very much high in principle. Considering the idea, we could design more efficient carbon-based oxygen electrocatalysts. Herein, we suggest that the basal plane can be utilized by introducing topological defects. The ORR mechanism and electronic structures were investigated to understand the intrinsic ORR activity of the topological defects and their activity origins via density functional theory calculations. Finally, we predicted that inversed Stone-Wales defect could be good ORR active sites.