

Unraveling Active Sites in Nitrogen-doped Defect Carbon for Bifunctional Oxygen Electrocatalysis

Qiu Jin

Department of Chemistry, University of Calgary, AB, Email: qiu.jin@ucalgary.ca

Nitrogen-doped carbon materials have attracted a great deal of attention as alternatives to precious metal-based catalysts for oxygen reduction reaction (ORR) and oxygen evolution reaction (OER). Previous studies show that defects in graphene layers are responsible for the high activity of carbon-based materials [1]. Herein, we investigate the effects of high concentration nitrogen-doping and defects in carbon nanosheets on the performance of ORR and OER using density functional theory (DFT) calculations. We find the possible active sites that largely boost the catalytic activities of the ORR and OER. This work sheds lights on the design of multifunctional metal-free materials.

[1] To, J. et al. High-performance oxygen reduction and evolution carbon catalysis: From mechanistic studies to device integration. *Nano Res.* **10**, 1163-1177 (2017).