Design Principles of Heteroatom-Doped Carbon-Based Electrocatalysts for Clean Energy Conversion

Lin C.,[1] Zhao Z.,[1] and Xia Z.H.[1,2]

[1] *Department of Materials Science and Engineering, University of North Texas, Deton, Texas,* USA

[2]*College of Energy, Beijing University of Chemical Technology, Beijing, China*

Clean and sustainable energy technologies, such as fuel cells, metal-air batteries, water-splitting and solar cells, are currently under intensive research and development because of their high efficiency, promising large-scale applications, and virtually no pollution or greenhouse gas emission. At the heart of these energy devices, there are three critical chemical reactions: *oxygen reduction reaction* (ORR), *oxygen evolution reaction* (OER) and *hydrogen evolution reaction* (HER) that determine the efficiencies of energy conversion and storage. These reactions, however, are sluggish and require noble metals (*e.g.*, platinum) or their oxides as catalysts. The limited resources and high cost of platinum have hampered the commercialization of these technologies. Therefore, it is necessary to search for alternative materials to replace Pt. Carbon nanomaterials, such as carbon nanotubes (CNTs) and graphene, are appealing as an alternative for metal-free catalytic applications because of their structures and excellent properties. Although the superior catalytic capabilities of heteroatom-doped carbon nanomaterials for ORR have been demonstrated, trial-and-error approaches are still used to date for the development of highly-efficient catalysts. To rationally design a catalyst, it is critical to understand which intrinsic material characteristics, or descriptors that control catalysis. Through first-principles calculations, we have identified a material property that serves as the activity descriptor for predicating ORR and OER activities, and established a volcano relationship between the descriptor and the bifunctional activities of the carbon-based nanomaterials. Such descriptor enables us to design new metal-free catalysts with enhanced ORR and OER activities, even better than those reported for platinum-based metal catalysts. The design principles can be used as a guidance to develop various new carbon-based materials for clean energy conversion and storage.[1-3]

[1] Z. Zhao, M. Li, L. Zhang, L. Dai, Z. Xia, *Advanced Materials*, **27**, 6834–6840 (2015).
[2] C. Lin, L. Zhang, Z. Zhao, Z.Xia, *Advanced Materials*, 29, 1606635 (2017)
[3] J. Zhang, Z. Zhao, Z. Xia, and L. Dai, *Nature Nanotechnology*,10, 444–452(2015).

Email: zhenhai.xia@unt.edu