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Abstract View Online

Rational Design of Novel Carbon Catalysts for Clean Energy Conversion and Storage

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Abstract

In fuel cells and metal-air batteries, there are critical chemical reactions: oxygen reduction reaction (ORR), and oxygen evolution reaction (OER), respectively. These reactions, however, are sluggish and require noble metals (e.g., platinum) or their oxides as catalysts. The scarcity and high cost of noble metals have hampered the commercial applications of these technologies [1]. 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 correlate intrinsic material characteristics with catalytic activities. Through first-principles calculations, we have identified a material property that serves as the activity descriptor for both ORR and OER, and established a volcano relationship between the descriptor and the catalytic activities of the carbon-based nanomaterials [2]. The design principles can be used as a guidance to develop various new carbon-based materials for clean energy conversion and storage.

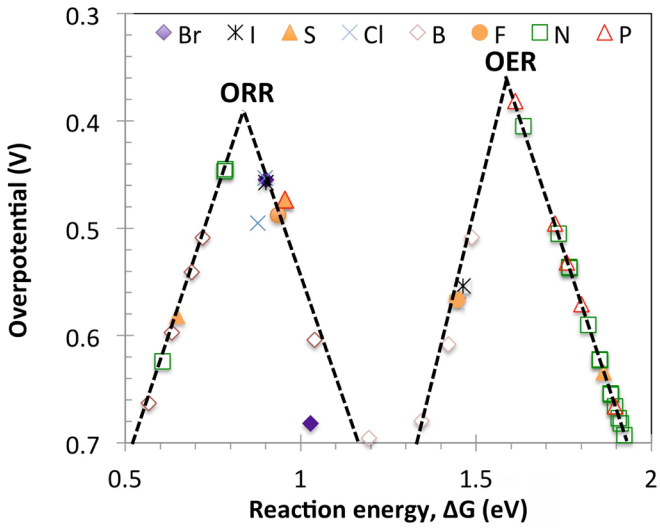

Figure 1. *Volcano relationships between the descriptor and the catalytic activities of the carbon-based nanomaterials.*

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