Pentagon defect in Carbon for Oxygen reduction reaction

Guoping Chen

International Institute for Carbon-Neutral Energy Research (I2CNER) Kyushu University,

744 Motooka, Nishi Ward, Fukuoka 819-0395, Japan.

The oxygen reduction reaction (ORR) is a fundamental electrochemical process central to the operation of energy conversion and storage technologies, particularly in devices like fuel cells and metal-air batteries. While platinum-based catalysts have historically been effective for ORR, their high cost and limited stability in acidic environments drive the search for alternative, more sustainable catalysts. Carbon-based materials have emerged as some of the most promising candidates for ORR catalysis due to their abundance, low cost, and tunable electronic properties. Numerous studies have aimed to clarify the catalytic roles of active carbon. [1] This research has extended to include dopants in carbon matrix and gradually to defect-rich carbon materials without dopants. Through extensive experimental studies and density functional theory (DFT) calculations, it is now widely recognized that the activation of carbon is driven by the asymmetric redistribution of charge and/or spin densities in carbon atoms near both dopants and defects.

Defects such as pentagons and vacancies have also been reported to create active sites for ORR. These defects can promote charge redistribution on π-conjugated carbon atoms. However, further studies are needed to understand the catalytic behavior of defects-including carbon catalysts, in which a critical aspect often overlooked in previous studies is the role of electron spin in the defect structure. In ORR catalysis, the interaction of electron spins can significantly influence the energy levels because the activation of the ground state triplet O_2 can be induced by the electrons from the catalyst with high spin concentrations. These unpaired electrons are central to facilitating electron transfer processes. Nonetheless, unlike transition metal-based catalysts, considerably less work has been done to exploit the spin properties in carbon materials with defects since inducing high spin concentrations in carbon matrix systems remains quite challenging. The introduction of pentagon defects has been proposed as a method to induce magnetism, thereby altering spin density and distribution in carbon-based materials. This suggests a promising strategy: creating active carbon sites with spin electrons by integrating a high concentration of pentagon defects. [2]

This presentation explores the specific roles of pentagon defects in carbon and their potential to advance ORR catalytic processes.

Reference:

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2. Chen, G.; Isegawa, M.; Koide, T.; Yoshida, Y.; Harano, K.; Hayashida, k.; Fujita, S.; Takeyasu, K.; Ariga, K.; Nakamura, J., Pentagon‐Rich Caged Carbon Catalyst for the Oxygen Reduction Reaction in Acidic Electrolytes. *Angew. Chem. Int. Ed.* **2024**, e202410747.