Unveiling the high activity origin of single atom iron catalysts for oxygen reduction reaction

With the support by the National Natural Science Foundation of China for Distinguished Young Scholars, the research team directed by Prof. Cao DaPeng (曹达鹏) at the State Key Laboratory of Organic-Inorganic Composites & College of Chemical Engineering, Beijing University of Chemical Technology, and the School of Materials Science and Engineering, Beihang University, recently reported the origin of high-ORR activity of single atom Fe catalysts, which was published in *PNAS* (2018, 115: 6626—6631).

Developing an efficient nonprecious-metal electrocatalyst to replace the Pt-based catalysts for oxygen reduction reaction (ORR) is still a grand challenge, because the extreme dependence of ORR on Pt-based catalysts severely hinders their commercial applications. Metallic single atom catalysts (SACs) have been considered as an ideal candidate, because SACs provide the maximum atomic efficiency and possess the refined M-N-C configuration (M = Fe, Co, Ni, etc.), which also offers an opportunity to explore the origin of high catalytic activity of SACs.

Cao's group proposed a surfactant-assisted method to synthesize single atom Fe catalysts supported on N-doped carbons (SA-Fe/NG). The SA-Fe/NG catalyst possesses extremely outstanding catalytic activities for ORR in both acidic and alkaline media. Impressively, the SA-Fe/NG-based acidic proton exchange membrane fuel cell (PEMFC) exhibits a high power density of 823 mW cm^{-2}. Combining experimental results and DFT calculations, they for the first time reveal that the origin of high-ORR activity of SA-Fe/NG is from the Fe-pyrrolic-N species, because such a molecular incorporation is the key to leading to the active site increase in an order of magnitude which successfully clarifies the bottleneck puzzle of why a small amount of iron in the SA-Fe catalysts can exhibit extremely superior ORR activity.

These findings may provide new insight into the origin of high-ORR activity of SACs, and also offer a universal surfactant-assisted method to develop highly efficient SACs.

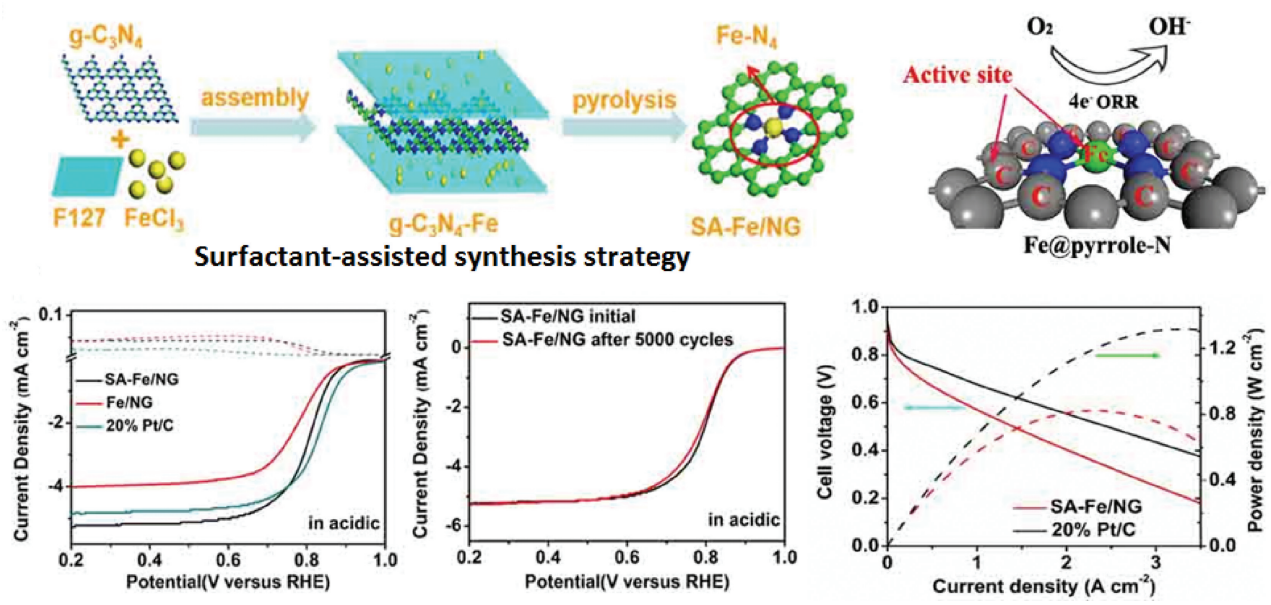

Figure A universal surfactant-assisted synthesis method, active sites and ORR properties of SA-Fe/NG catalysts, and performance of PEMFC.