# Researchers realize efficient hydrogen-peroxide production in acid

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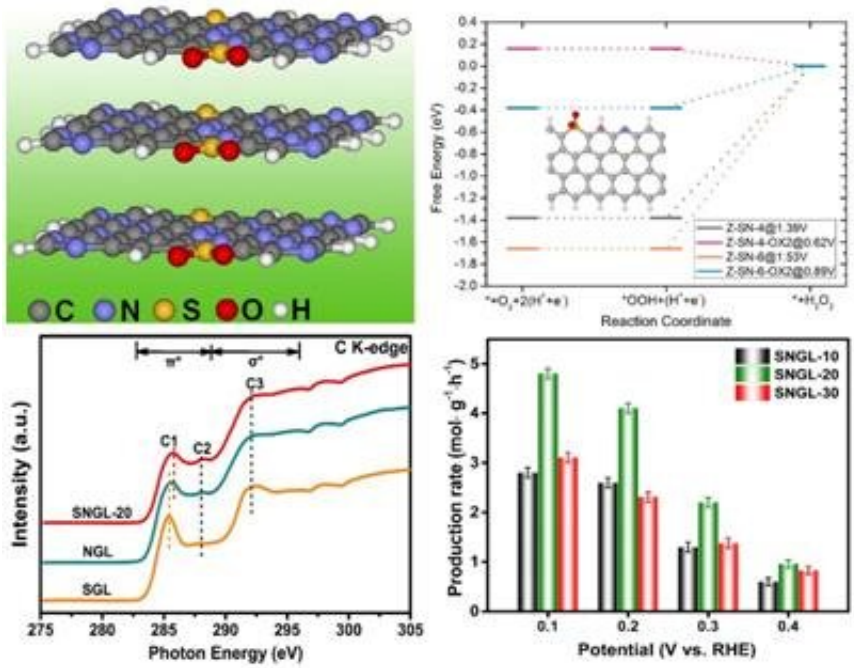


Illustration of the research. Credit: Prof. Guan's Group

As one of the 100 most important chemicals in the world, hydrogen peroxide ($H_2O_2$) is mainly produced by the energy- and waste-intensive anthraquinone oxidation (AO) method. Replacing the AO method with a more environmentally-benign electrochemical two-electron oxygen reduction reaction ($2e^-$ ORR) depends on cheap and efficient catalysts.

However, metal-free, carbon-based catalyst as a promising candidate

behaves encouragingly only under neutral or alkaline conditions, where $H_2O_2$ is unstable for collection or unfavorable for linking applications, i.e., the e-Fenton reaction. Moreover, it remains challenging to identify the real active catalytic sites and the underlying $2e^-$ ORR mechanism.

In a study published in *Chem Catalysis*, a research group led by Prof. Guan Lunhui from the Fujian Institute of Research on the Structure of Matter of the Chinese Academy of Sciences developed a metal-free, highly efficient acidic $2e^-$ ORR catalyst with recorded hydrogen peroxide production rate based on pyrimidine-assisted active site modulation and S, N-codoped few-layered graphene for valence electronic optimization.

The catalyst exhibited exceptional activity and selectivity for $2e^-$ ORR in acid. The $H_2O_2$ selectivity reaches 90%~100% over a potential range of 0.20~0.55 V and the maximum $H_2O_2$ production rate (4.8 $mol \cdot g^{-1} \cdot h^{-1}$) exceeds all the reported $H_2O_2$ production performance for carbon material-based catalysts.

Experiments and density-functional-theory simulations (contributed by Prof. Chai Guoliang) revealed that the synergy effect of the combined oxidized sulfur and pyridinic-N functional motif can lower the Fermi level of valence electronic states of active edge carbon sites, and thus leads to suitable binding strength of *OOH intermediate for high selectivity and performance $2e^-$ ORR for $H_2O_2$ formation.

In particular, the researchers observed an obvious peak-shift to high energy of C 1s excitation in near edge X-ray absorption fine structure with S incorporation, as solid evidence for the valence electronic optimization of carbon catalyst surface.

In addition, coupled with Fenton reaction for an electron-Fenton process, it can degrade a model organic pollutant (methylene blue [MB], 50 ppm)

to colorless in a short time of 15 min.

This study not only creates an efficient carbon-based catalyst for $H_2O_2$ production in acid, but also provides a useful electronic property optimization route for future tuning of carbon-based materials catalysts.

**More information:** Jiaoxing Xu et al, Pyrimidine-assisted synthesis of S, N-codoped few-layered graphene for highly efficient hydrogen peroxide production in acid, *Chem Catalysis* (2022). DOI: 10.1016/j.checat.2022.04.011

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