Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

The identification of active N species in N-doped carbon carriers which improves the activity of Fe electrocatalysts towards oxygen evolution reaction

Ziwu Liu,* JiaJia, Fei Han, Guo-Jun Kang, Ling Liu, Jinlong Liu and Quan-De Wang*

Supporting Figures

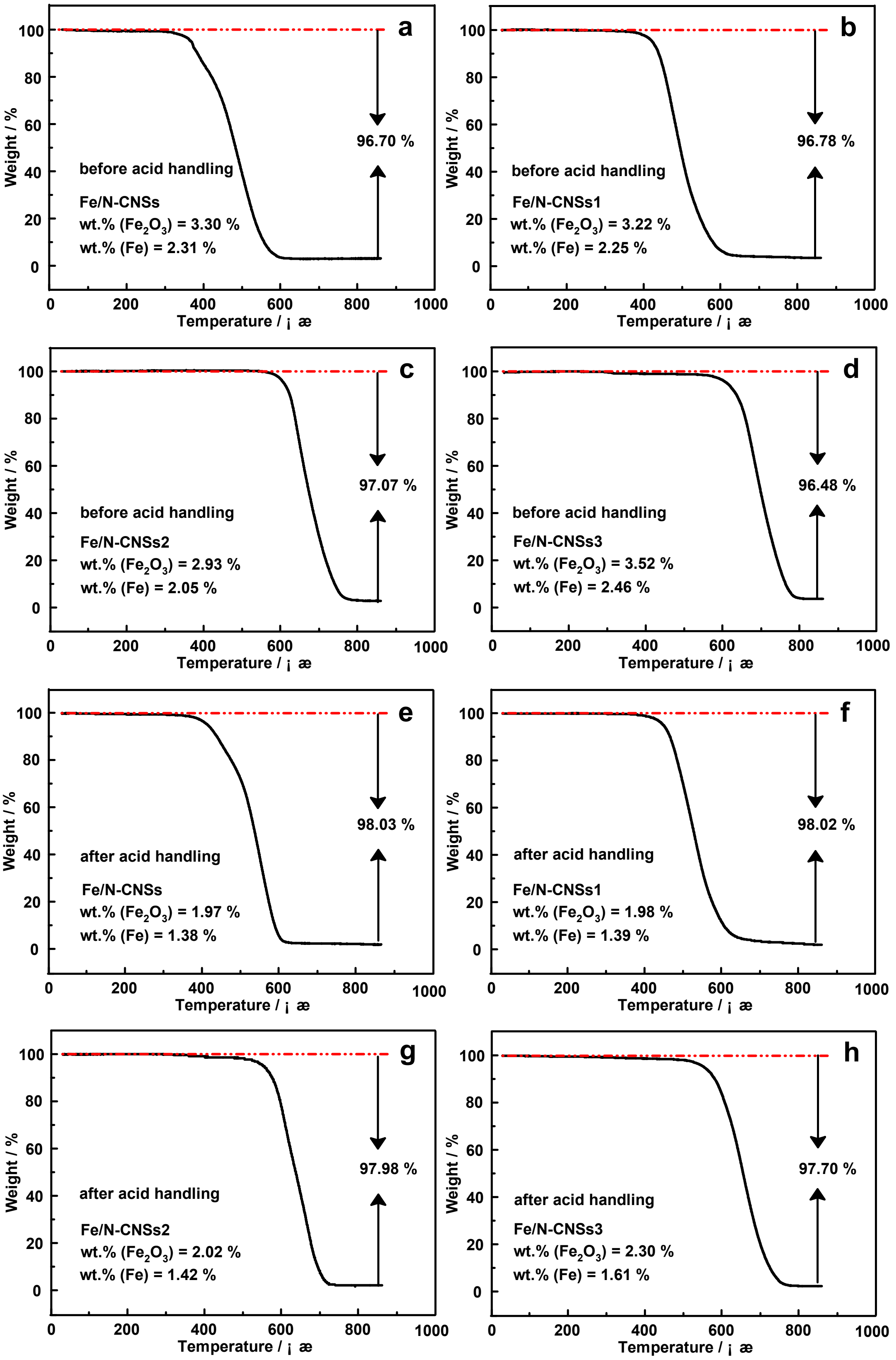

Fig. S1. The TG curves of Fe/N-CNSs, Fe/N-CNSs1, Fe/N-CNSs2 and Fe/N-CNSs3 before and after acid handling.

From Fig. S1, it can found that Fe/N-CNSs, Fe/N-CNSs1, Fe/N-CNSs2 and Fe/N-CNSs3 began to lose their weight drastically at 302, 379, 560 and 559 ℃, respectively, indicating that the stability of samples would increase when they were handled at high temperature.

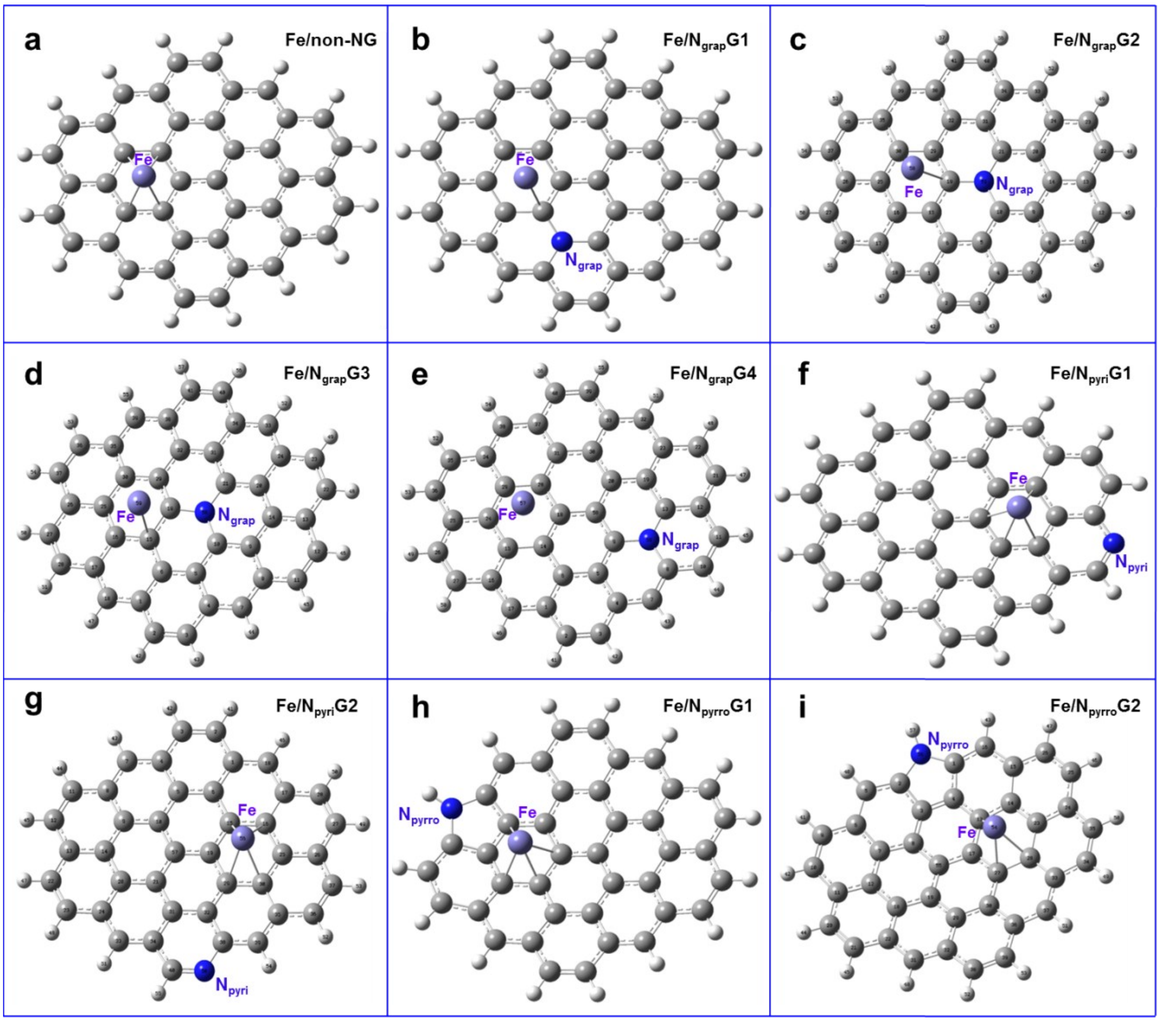

Fig. S2. Nine stable configurations: a) Fe/non-NG, b) Fe/N$_{\mathrm{grap}}$G1, c) Fe/N$_{\mathrm{grap}}$G2, d) Fe/N$_{\mathrm{grap}}$G3, e) Fe/N$_{\mathrm{grap}}$G4, f) Fe/N$_{\mathrm{pyri}}$G1, g) Fe/N$_{\mathrm{pyri}}$G2, h) Fe/N$_{\mathrm{pyrro}}$G1 and i) Fe/N$_{\mathrm{pyrro}}$G2.

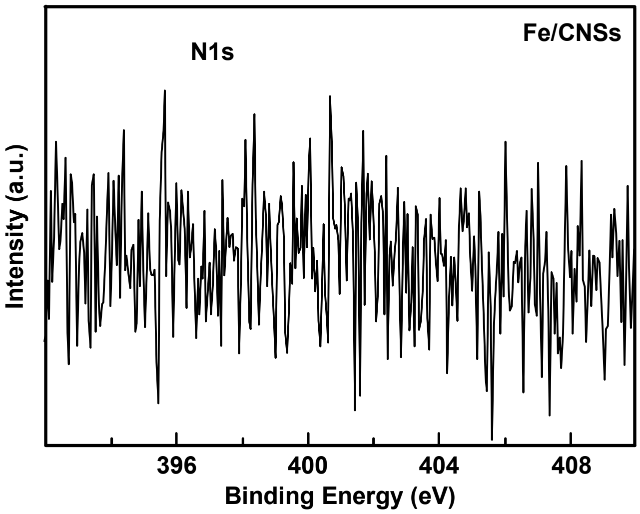

Fig. S3. The high-resolution N1s XPS spectra of Fe/CNSs synthesized at 1500 °C for 3 h under a vacuum condition (vacuum degree: -1).

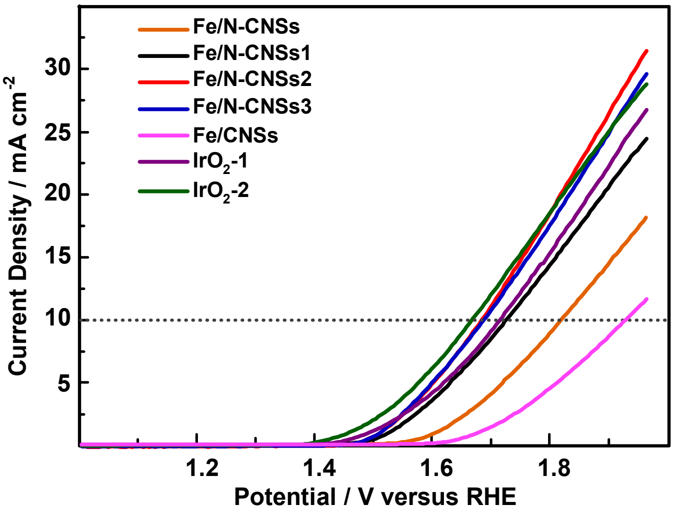

Fig. S4. The OER polarization curves of Fe/CNSs, Fe/N-CNSs, Fe/N-CNSs1, Fe/N-CNSs2, Fe/N-CNSs3 and IrO_2 in N_2-saturated 0.1 M KOH solution at the rotation rate of 1600 rmp.

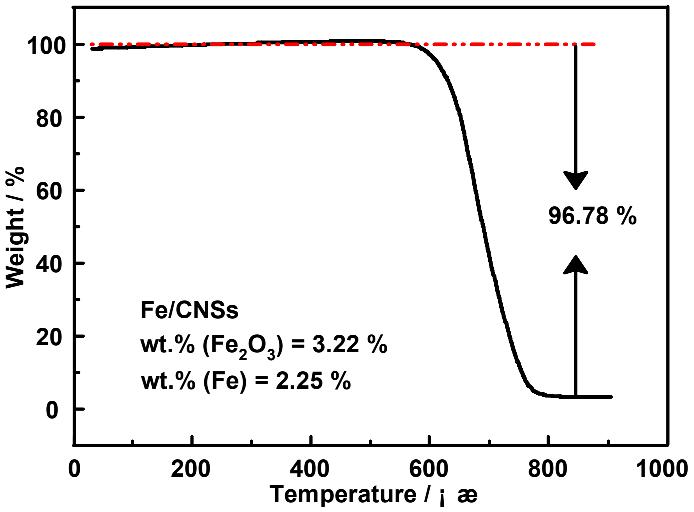

Fig. S5. The TG curve of Fe/CNSs synthesized at 1500 °C for 3 h under a vacuum condition through the method in experimental section.

To investigate the possible influence of oxygen on the identification of active N species, we prepared the Fe/CNSs without any N species at 1500 °C for 3 h under a vacuum condition and estimated its OER activity through the methods described in experimental section in our manuscript. From the XPS spectra of Fe/CNSs in Fig. S3, it could be found that all N species were removed from the Fe/CNSs. Meanwhile, Fig. S4 showed that the OER activity of Fe/CNSs (O: ca. 3.98 at.%; Fe: ca. 2.25 wt.%, Fig. S5) was much inferior to those of four Fe/N-doped CNSs catalysts, demonstrating that the doping of N species could enhance the OER activity of Fe greatly and the existence of oxygen does not influence obviously the identification of active N species in this work.

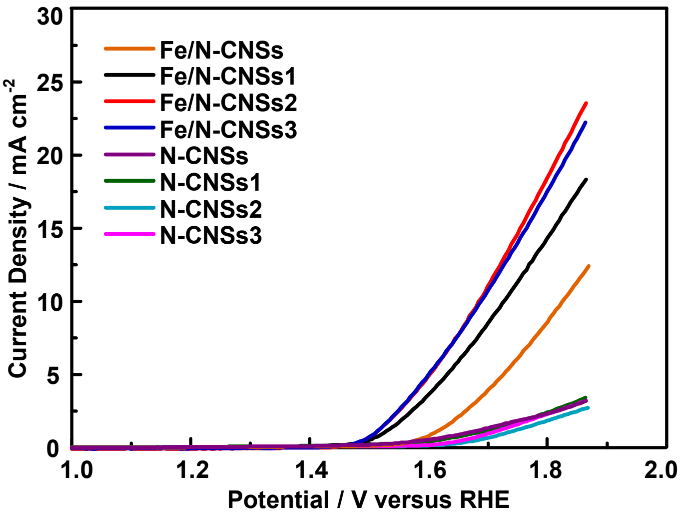

Figure S6. The OER activities of four samples before and after acid handling.

To eliminate the possible influence of the pyridine N, pyrrolic N and graphitic N in carbon nanospheres on the OER activity of our prepared Fe-based catalysts in this work, we dissolved iron from the surface of Fe/N-CNSs, Fe/N-CNSs1, Fe/N-CNSs2 and Fe/N-CNSs3 by concentrated hydrochloric acid under ultrasonic wave for 3 h and estimated their OER activities in the potential range of 1.0 to 1.865 V in alkaline medium, respectively. As shown in Figure S6, the OER activities of pure N-CNSs, N-CNSs1, N-CNSs2 and N-CNSs3 with Fe removing from their surface all were much inferior to those of Fe/N-CNSs, Fe/N-CNSs1, Fe/N-CNSs2 and Fe/N-CNSs3, indicated that the pyridine N, pyrrolic N and graphitic N in carbon nanospheres did not provide large OER activity and Fe in these samples mainly served as active catalyst. So, pyridine N and pyrrolic N in carbon nanospheres would not obviously influence the identification of active N species which improve the Fe OER activity in this work.