catalysts

Supplementary Materials: Reduction Process of Iron Catalyst Precursors for Ammonia Synthesis Doped with Lithium Oxide

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Received: 20 September 2018; Accepted: 16 October 2018; Published: date

The reduction of the industrial catalyst precursor KAT-K_2O was examined in-situ under isothermal conditions at a temperature of t=470 °C. Results are shown in (Figures S1,S2).

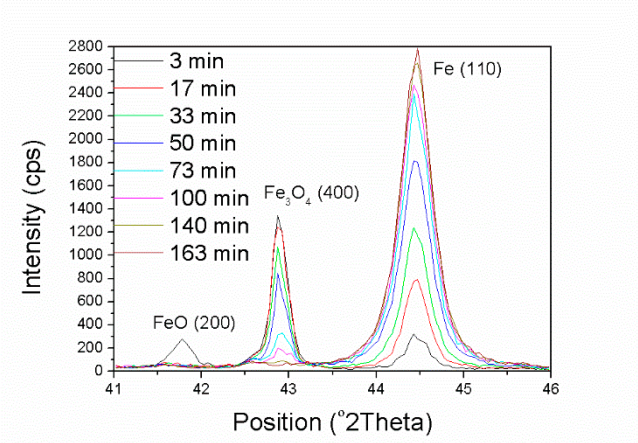

Figure S1. Demonstration X-ray patterns of the industrial catalyst precursor KAT-K_2O taken after various reduction times at a temperature of 470 °C.

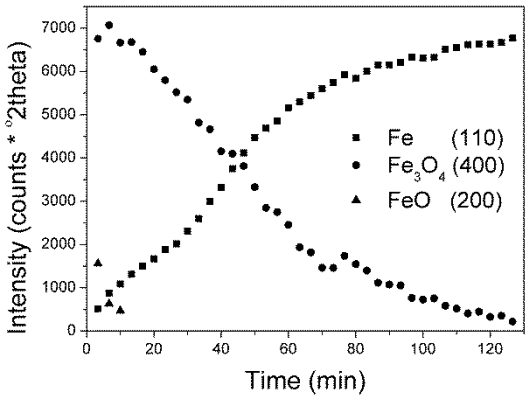

Figure S2. Dependence of peak intensities of Fe_3O_4, FeO, and Fe on the reduction time for the industrial catalyst precursor KAT-K_2O (T=470 °C). For better view the peak intensity of Fe phase was divided by 4.

In demonstration X-ray patterns, (Figure 1), the shift of Fe_3O_4 peaks are not noticeable. After the reduction process, only peaks belonging to the $CaFe_3O_5$ were detected. That phase does not undergo the full reduction.

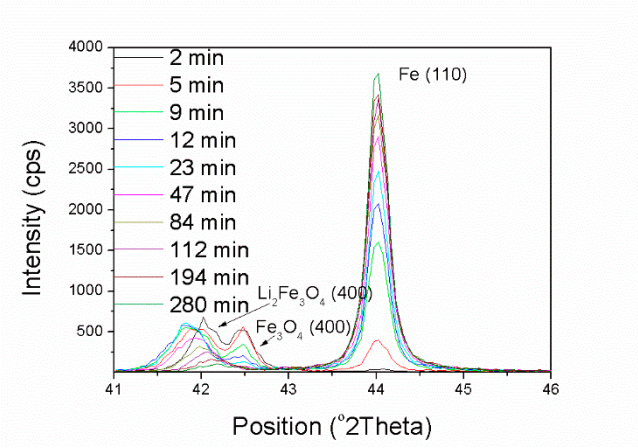

Figure S3. X-ray patterns taken after various times of KAT1-Li_2O catalyst precursor reduction at a temperature of 520 °C.

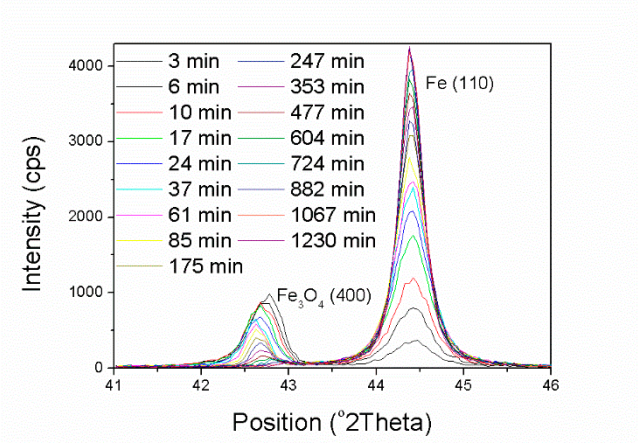

Figure S4. X-ray patterns of the KAT2-Li_2O catalyst after various time of the reduction at 520 °C.

In the early stage of the KAT2-Li_2O precursor reduction, asymmetry of the Fe_3O_4 phase peak, from a side of lower angles, is visible, which may suggest the occurrence of an additional phase (Figure 4).