

Supporting information

The Nature of the Selective Species in Fe-HZSM-5 for Non-Oxidative Methane Dehydroaromatization

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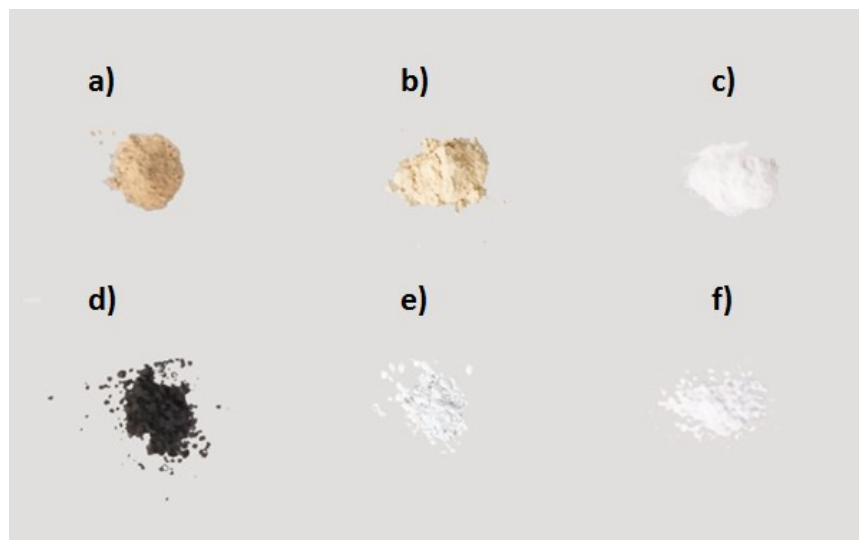


Figure S1. Powder samples of the three catalysts as synthesized: a) Fe@HZSM-5, b) Fe/HZSM-5, and c) H-(Fe)ZSM-5; and the same catalysts after H₂-TPR up to 1000°C: d) Fe@HZSM-5, e) Fe/HZSM-5, and f) H-(Fe)ZSM-5.

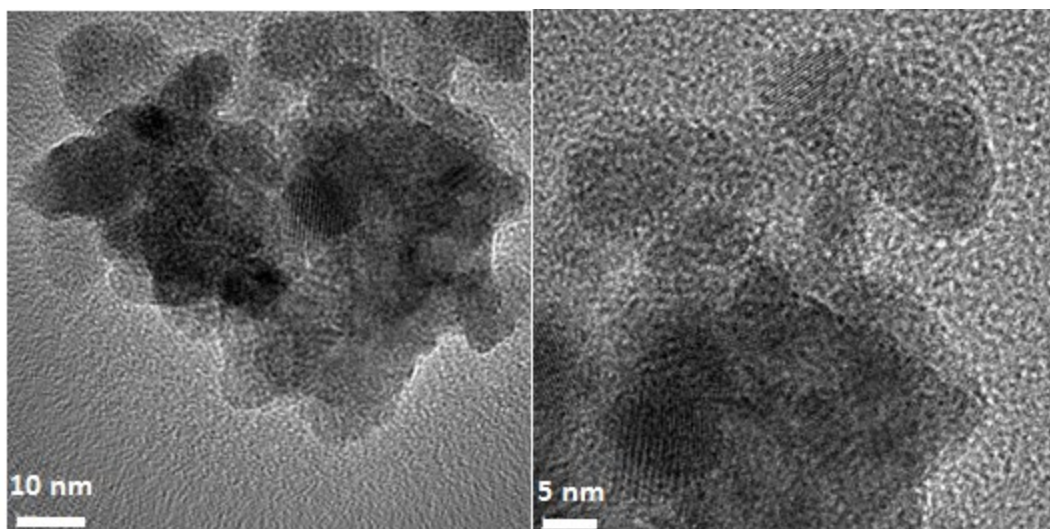


Figure S2. TEM for commercial Fe_2O_3 NPs.

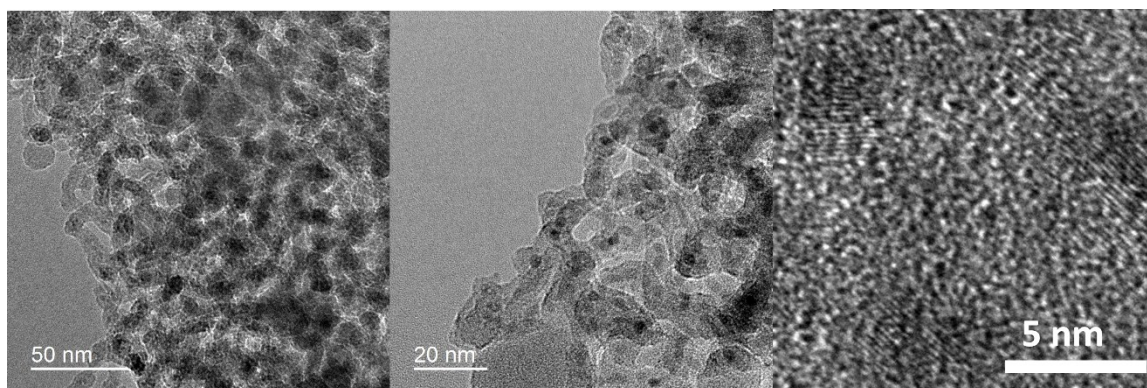


Figure S3. TEM images with different magnifications for the precursor of Fe@HZSM5 catalyst “ Fe@silica ”. While the structure of the silica matrix is fundamentally different from that of the HZSM-5 zeolite, the embedded Fe NPs are identical to those after conversion.

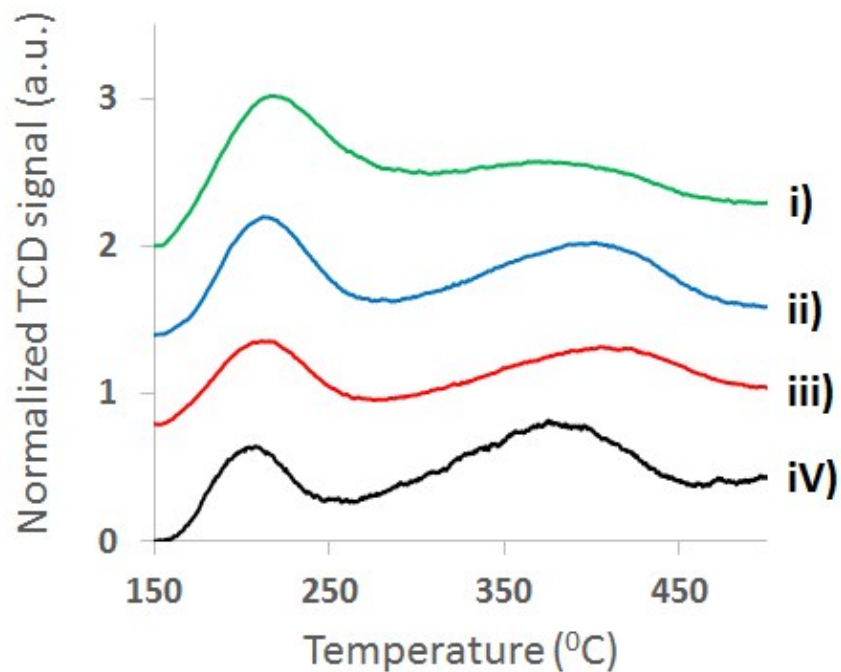


Figure S4. NH_3 -TPD profiles for i) Fe@HZSM-5, ii) H-(Fe)ZSM-5 iii) Fe/HZSM-5, and iv) parent HZSM-5.

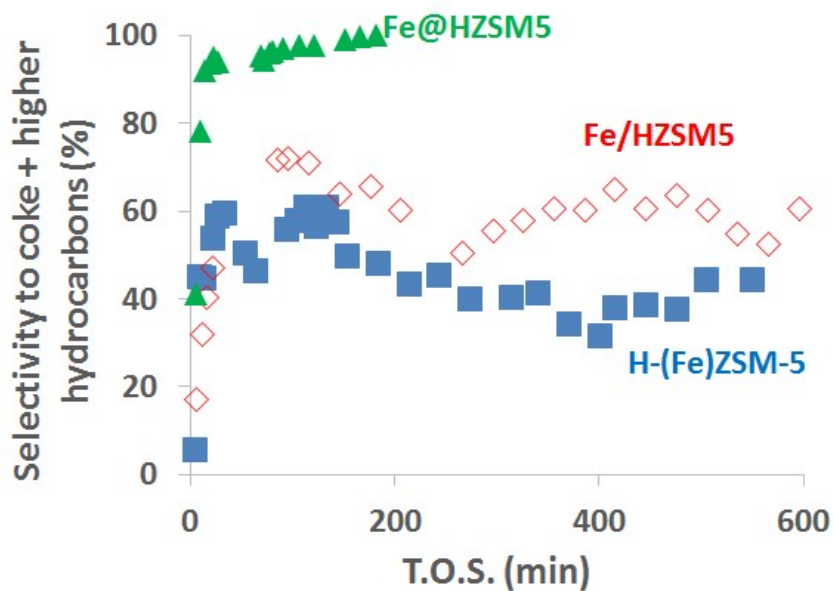


Figure S5. Selectivity towards higher hydrocarbons and coke for the three Fe-HZSM-5 catalysts at 700°C. GHSV: 3750 cc/g/h, calculated from a carbon balance at each time point. Note that while the experimental set-up did not allow detection of higher hydrocarbons, quantification of the carbon formation at the end of each experimental run (see table 3 in the main paper) suggests that the majority of the combined selectivity shown in the graph is coke selectivity.

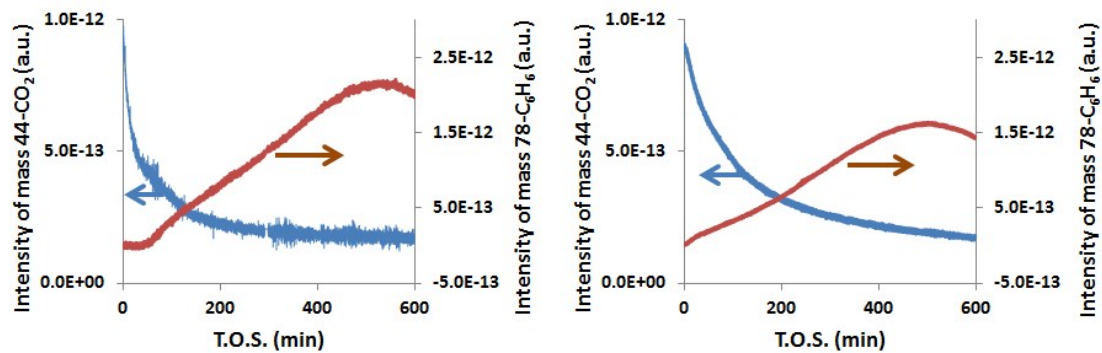


Figure S6. Mass spectroscopy data for the Fe/HZSM5 catalyst (left) and H-(Fe)ZSM-5 catalyst (right) at 700°C (GHSV: 3750 cc/g/h with 50% CH₄ and 50% He). Since oxygen can only be extracted from the Fe species in the reaction system, CO₂ observed over these two catalysts must result from reduction of Fe species.