Electronic Supplementary Information

Roles of the structural defects and the combined acidity of $H_3PW_{12}O_{40}$/Zr-MCM-41 catalysts in ultralow sulfur diesel production

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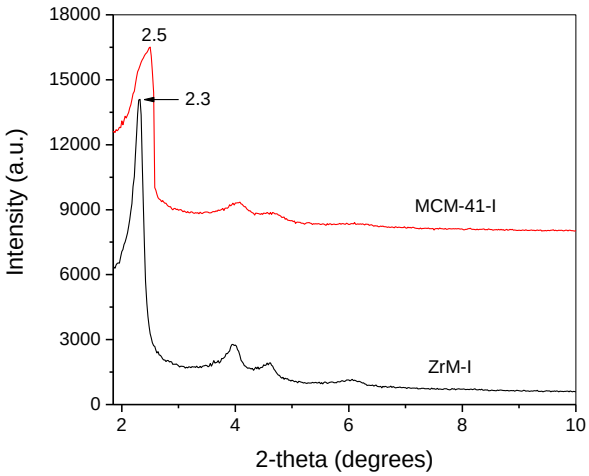
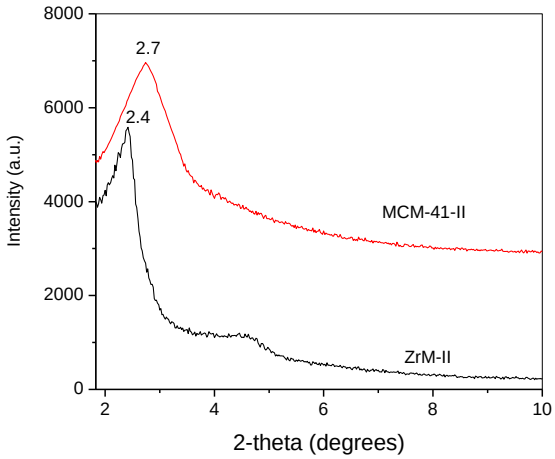
1. Low angle XRD analysis

In comparison with the XRD pattern of pure MCM-41-I and MCN-41-II samples, the (100) peak in the XRD patterns of the Zr doped ZrM-I and ZrM-II samples slightly shifts toward to the low two-theta region. This indicates that Zr^{4+} inserted into the structure of MCM-41 (SI Figures 1 and 2).



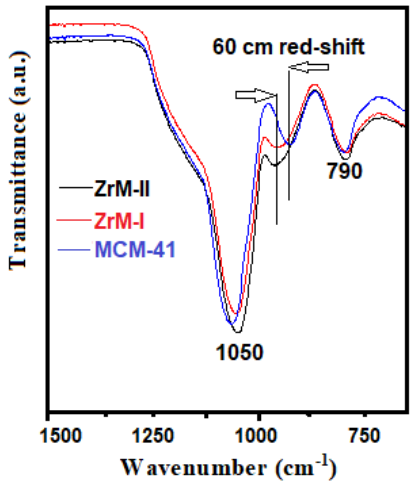
SI Figure 1. Low angle XRD patterns of MCM-41-I and Zr-MCM-41-I (ZrM-I). Fumed silica was used as Si precursor and tetrabutylammonium hydroxide (TBAOH) aqueous solution as precipitating agent in the synthesis.



SI Figure 2. Low angle XRD patterns of MCM-41-II and Zr-MCM-41-II (ZrM-II). Tetraethylorthosilicate (TEOS) was used as Si precursor and $NH_3 \cdot H_2O$ (28 wt%) was used as precipitating agent.

2. FTIR characterization

We also performed the FTIR characterization (SI Figure 3), where it was found that the IR band at 920 cm^{-1} in MCM-41 red-shifts to 980 cm^{-1} approximately for both ZrM-I and ZrM-II samples, confirming that after Zr^{4+} doping, the Zr^{4+} inserted into the MCM-41 framework.



SI Figure 3. FTIR spectra of the MCM-41 and ZrM-I and ZrM-II samples