

Supporting Information

for

Encapsulation of Chiral Fe(salan) in Nanocages with Different Microenvironment for Asymmetric Sulfides Oxidation

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1. The TEM images of the nanocages

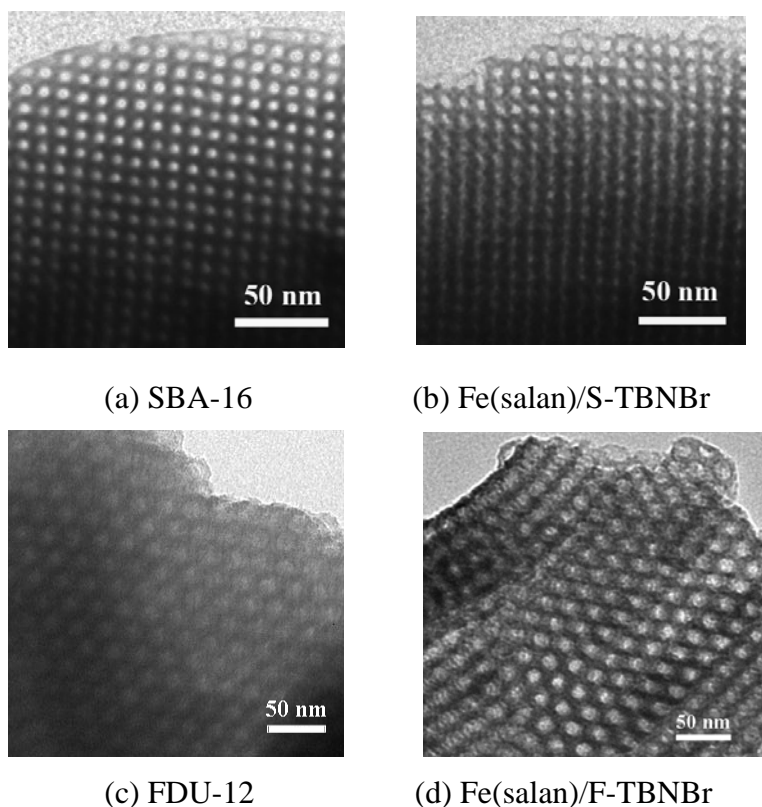


Fig. S1 The TEM images of SBA-16, FDU-12, Fe(salan)/S-TBNBr and Fe(salan)/F-TBNBr.

2. UV-vis spectra of the catalysts.

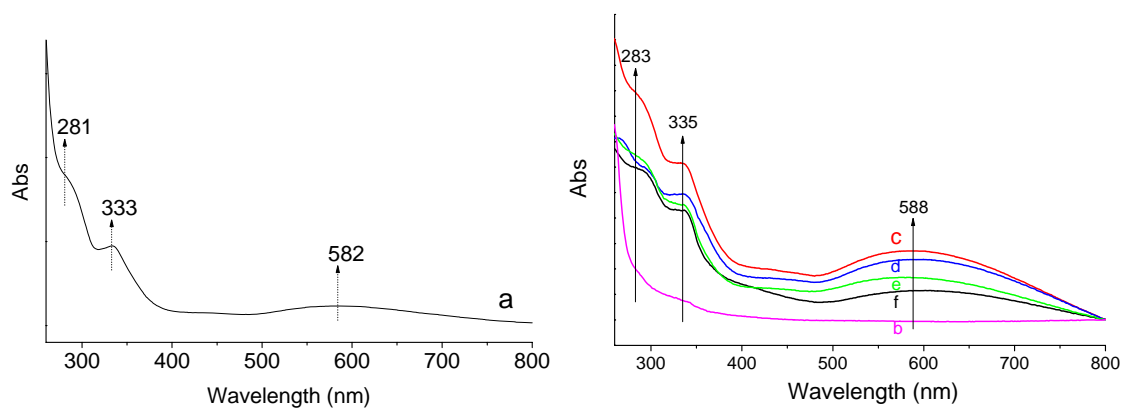


Fig. S2 UV-vis spectra of Fe(salan) in dichloromethane, and UV-vis diffusion reflectance spectra of silylated SBA-16 and the solid catalyst: (a) Fe(salan) in dichloromethane; (b) SBA-16-TBNBr; (c) Fe(salan)/S-TBNBr; (d) Fe(salan)/S-ILBr; (e) Fe(salan)/S-TBNCl; (f) Fe(salan)/S-C3.

3. Compared the gas adsorption of H₂O and benzene by the fresh catalyst Fe(salan)/S-TBNBr with the recovered catalyst Fe(salan)/S-TBNBr.

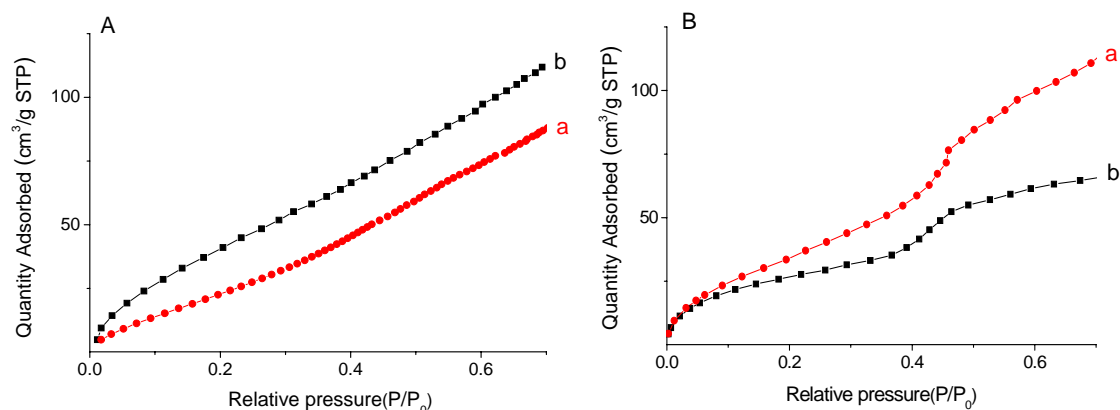


Fig. S3 The gas adsorption of H₂O (A) and benzene (B) with the solid catalysts: (a) Fresh catalyst Fe(salan)/S-TBNBr; (b) Recovered catalyst Fe(salan)/S-TBNBr

4. Determining the pore entrance size of the nanocage by the adsorption experiment.

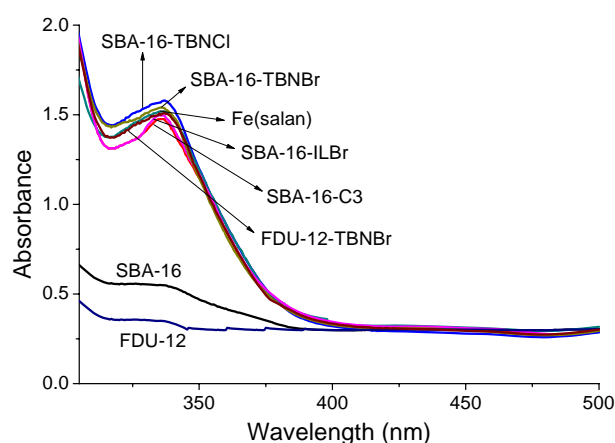


Fig. S4 UV-vis spectra of Fe(salan) solution before and after adsorption with SBA-16, FDU-12 and silylated SBA-16 and FDU-12.

The pore entrance size of SBA-16 and FDU-12 before and after modification with different silylation agents was detected using Fe(salan) as a probe molecule. 0.08 g of the organically modified SBA-16-R or FDU-12-R was dispersed in 5 mL of chloroform containing 5.43×10^{-4} mmol of Fe(salan). After stirring for 5 h, the liquid was isolated by filtration and measured with a UV-vis spectrophotometer. As shown in Fig. S1, the absorbance intensity of the characteristic band of Fe(salan) in DCM after treatment with SBA-16 and FDU-12 dramatically decreased, suggesting that the pore entrance size of SBA-16 and FDU-12 is large

enough to allow the free diffusion of Fe(salan) into and out of the nanocage. This result is reasonable because the molecular size of Fe(salan) is 1.2×1.8 nm, while the pore entrance size of SBA-16 and FDU-12 is supposed to be 3-4 nm. After the solution was adsorbed with modified SBA-16-R and FDU-12-R, the absorbance intensities of the characteristic band of Fe(salan) in DMC remained almost the same, indicating that the pore entrance size of the samples is smaller than Fe(salan), which suggests that the current modification condition can prevent the encapsulated Fe(salan) from diffusion out of the nanocage.