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## **Supporting Information**

Figure S1- Nitrogen adsorption isotherms to determine the window size of SBA-16 materials after functionalization

SBA-16 materials were functionalized with organosilanes with different carbon chains. The samples were designated SBA-16 Cx, where x is the number of carbon on the carbon chain. For example, SBA-16A-373-5.5-C6 is SBA-16A-373-5.5 that was functionalized with n-hexyltriethoxysilane.



Figure S2- Nitrogen adsorption isotherms to determine the window size of m-MCF materials after functionalization

m-MCF materials were functionalized with organosilanes with different carbon chains. The samples were designated m-MCF Cx, where x is the number of carbon on the carbon chain.



Figure S3- SEM images of pristine materials (A) m-MCF-50, (B)m-MCF-60, (C)m-MCF-70 and (D) m-MCF-80 Scale Bars: 2µm



Figure S4- SEM images pristine materials (A) SBA16-A-373-5.5 (B) SBA16-A-373-24 (C)SBA16-B-353-24 (D)SBA16-C-373-24, scale bars: $2\mu$ m



## Figure S5- m-MCF-60 functionalized with n-propyl groups (left) and pristine m-MCF-60 (right) mixed with water.

Pristine m-MCF-60 was easily dispersed in water due to silanol groups on its surface. In the case of functionalized m-MCF-60, the silica did not disperse in water due to the hydrophobic groups grafted on its surface.



Figure S6-  $N_2$  physisorption of pristine material and the respective material functionalized with n-propyl groups



Figure S7-IR spectra (A) Functionalized MCF-60 with n-propyl groups (B) pristine m-MCF-60



Figure S8- TGA analysis of a pristine m-MCF and functionalized m-MCFs (top frame) and a pristine SBA-16 and functionalized SBA-16 (bottom frame)



Figure S9-N<sub>2</sub> Physisorption at 77K of m-MCF-60, F.m-MCF-60 and Fe.F.m-MCF-60

Table S1- Structural properties of pristine, functionalized and after encapsulation of Fe
salen

Material	Surface area (m²/g)	Pore volume (cm <sup>3</sup> /g)	Cage size (nm)
m-MCF-60	623	0.66	16.5
F-m-MCF-60	313	0.41	16
Fe-F-m-MCF-60	242	0.22	15



Figure S10- XRD analysis of fresh and spent Fe(salen) F.m-MCF-70



Figure S11- 1H NMR spectra of salen ligand

## Table S2- Recyclability of Fe(salen) immobilized in F.m-MCF-60 for the oxidation of thioanisole



1a

1b

Run	Conversion (%)	Selectivity (%)	ee (%) <sup>a</sup>
1	90	99	57
2	80	99	0
3	75	98	0
4	69	97	0
5	63	98	0

Determined with GC-FID, selectivity to 1a, <sup>a</sup> determined by chiral HPLC analysis, Reaction conditions: 4 mL of solvent, 0.4 mmol of thioanisole, oxidant (0.65 mmol) and catalyst (1 mol% Fe), 20°C, 4 hours



Figure S12- Time-conversion plot and leaching test as evidence for the nature of the catalyst for sulfoxidation of benzyl phenyl sulfide