

## Supporting Information

### **Binuclear TiOMn Charge-Transfer Chromophore in Mesoporous Silica**

Xuini Wu, Walter W. Weare, and Heinz Frei\*

Physical Biosciences Division, Lawrence Berkeley National Laboratory,

University of California, Berkeley, CA 94720

[HMFrei@lbl.gov](mailto:HMFrei@lbl.gov)

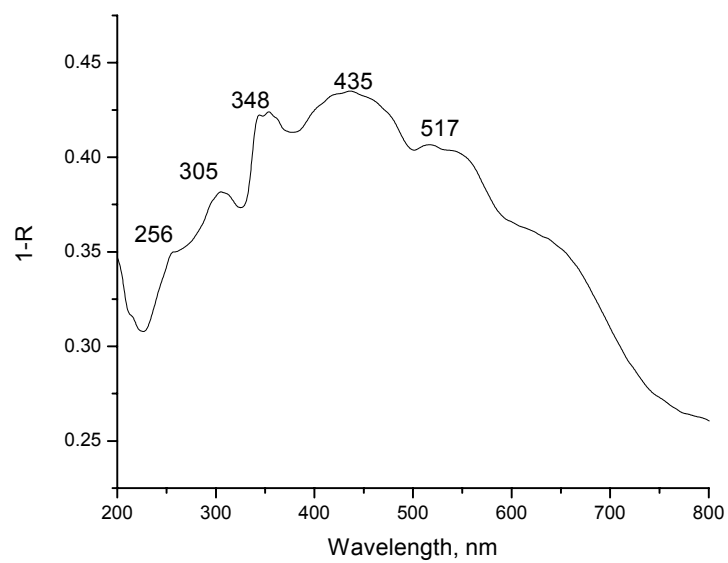


Figure S1: UV-Visible diffuse reflectance spectrum (DRS) of  $\text{Mn}(\text{NCCH}_3)_2\text{Cl}_2$  mixed with MCM-41.

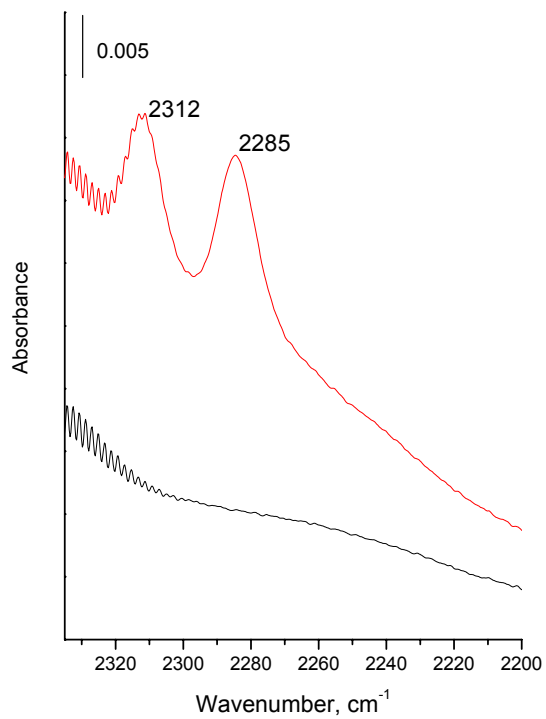


Figure S2: FT-IR of  $\text{Mn}(\text{NCCH}_3)_2\text{Cl}_2$  mixed with MCM-41.

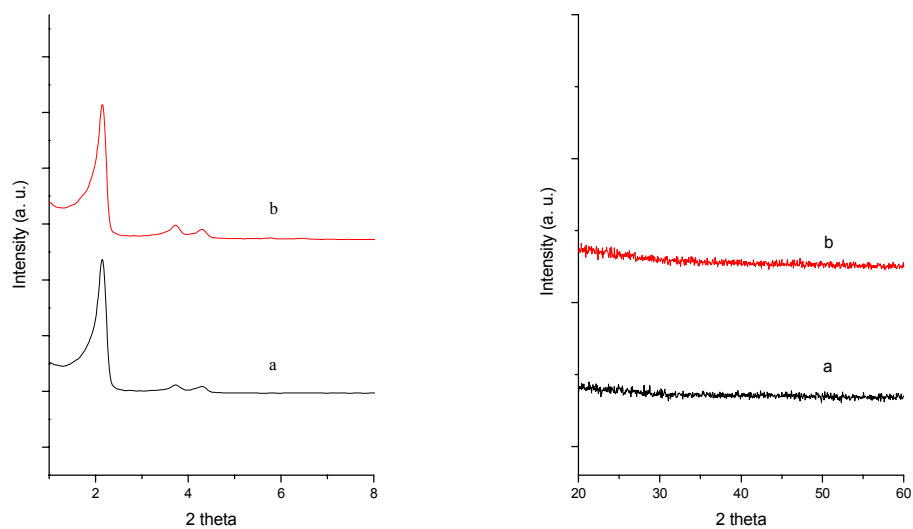


Figure S3: Powder XRD of Mn-MCM-41-as-synthesized (a) and Mn-MCM-41-vacuum at 350°C (b).

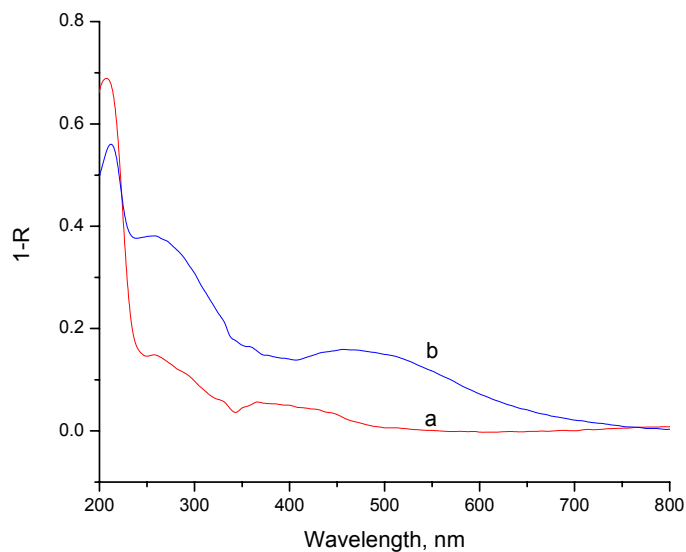


Figure S4: (a) DRS of  $(\text{Et}_4\text{N})_2\text{MnCl}_4$  (wt 2%) mixed with MCM-41.  
(b) DRS of Mn-MCM-41 grafted using  $(\text{Et}_4\text{N})_2\text{MnCl}_4$  as precursor.

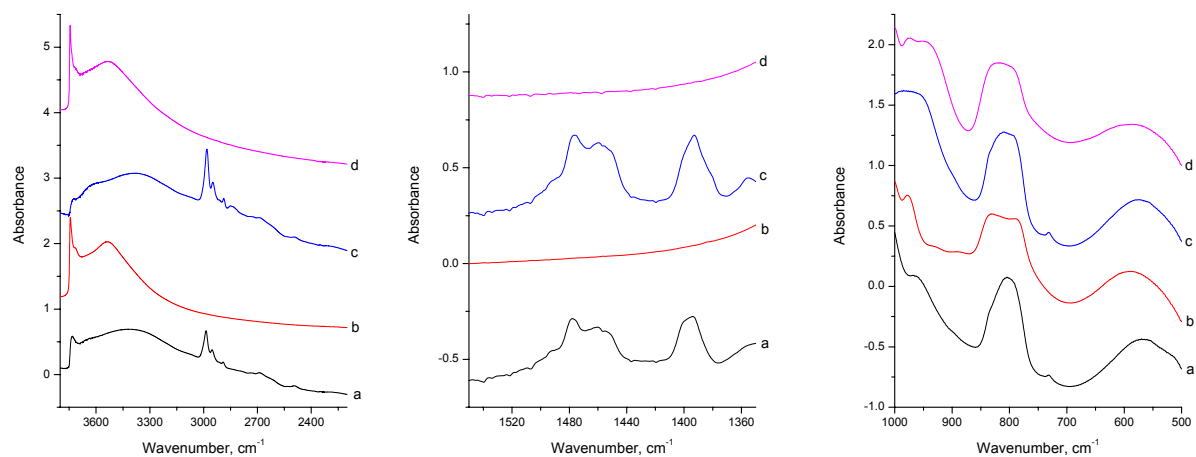
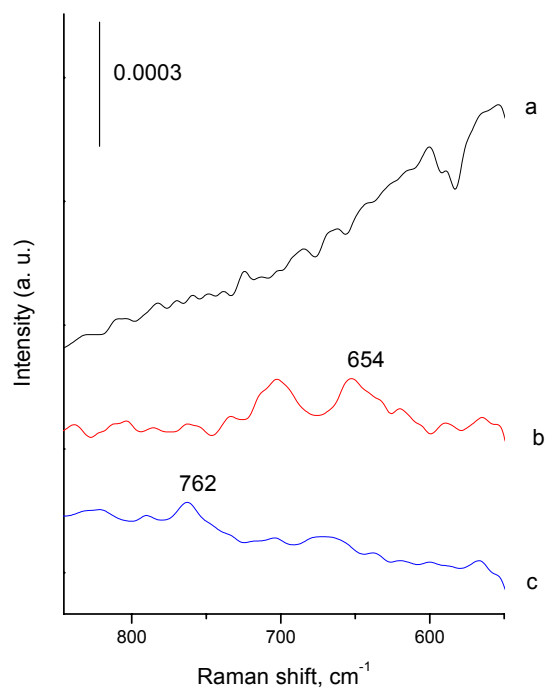
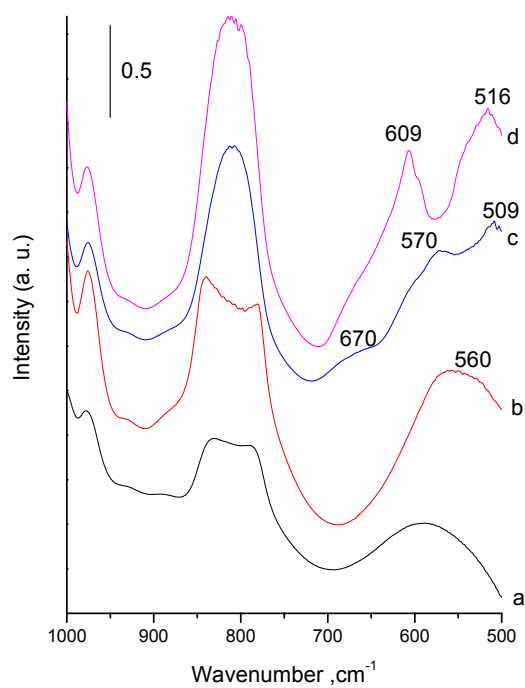


Figure S5: FTIR difference spectra of a) Mn-MCM-41-as-synthesized; b) Mn-MCM-41 heated under vacuum at 350 °C; and c) TiMn-MCM-41-as-synthesized; (d) TiMn-MCM-41 heated under vacuum at 350 °C.

(A)



(B)



(C)

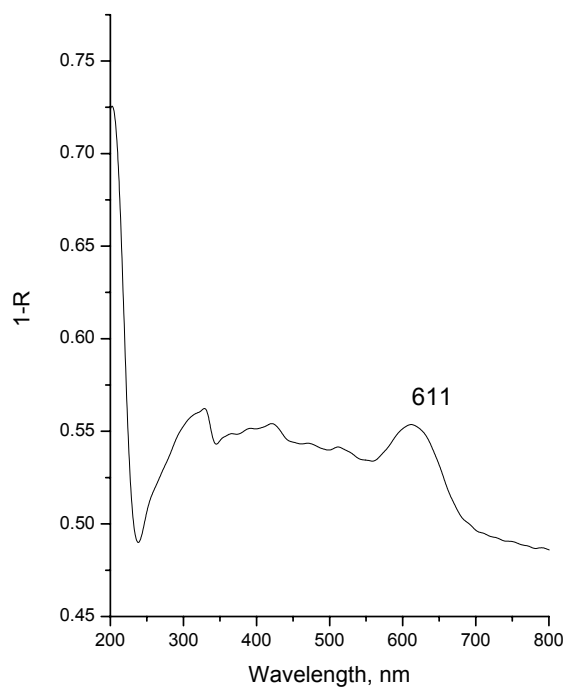


Figure S6: A. FT-Raman spectra of (a) Mn-MCM-41, (b) Mn<sub>2</sub>O<sub>3</sub> (wt 2%) mechanically mixed with MCM-41, (c) MnO (wt 2%) mechanically mixed with MCM-41.

B. FT-IR spectra of (a) Mn-MCM-41, (b) MnO (wt 2%) mechanically mixed with MCM-41, (c) Mn<sub>2</sub>O<sub>3</sub> (wt 2%) mechanically mixed with MCM-41, (d) Mn<sub>3</sub>O<sub>4</sub> (wt 2%) mechanically mixed with MCM-41.

C. DRS of MnO (wt 2%) mechanically mixed with MCM-41.

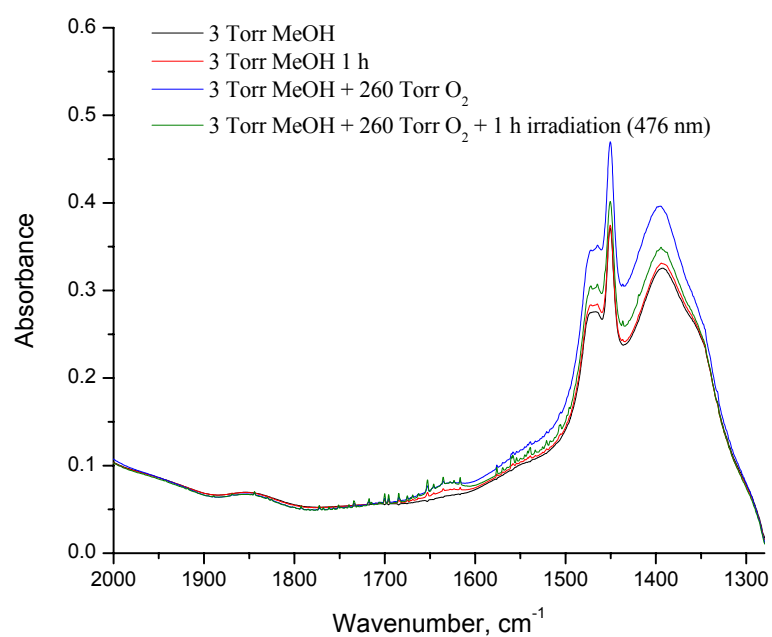


Figure S7: Infrared difference spectra of Ti-MCM-41 upon 3 Torr methanol loading, after 1 h waiting in the dark, after loading of 260 Torr O<sub>2</sub>, and 476 nm irradiation for 1 h.