Electronic Supplementary Information for Dalton Transactions

Supporting Information

Binuclear TiOMn Charge-Transfer Chromophore in Mesoporous Silica

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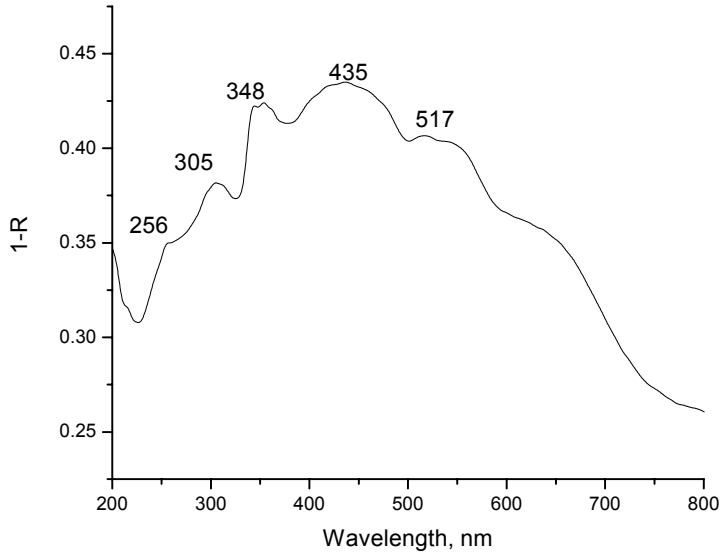


Figure S1: UV-Visible diffuse reflectance spectrum (DRS) of $Mn(NCCH_3)_2Cl_2$ mixed with MCM-41.

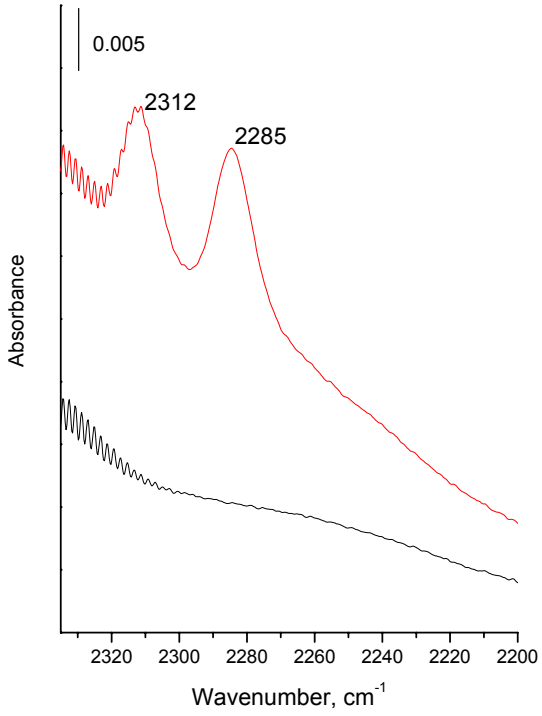


Figure S2: FT-IR of $Mn(NCCH_3)_2Cl_2$ mixed with MCM-41.

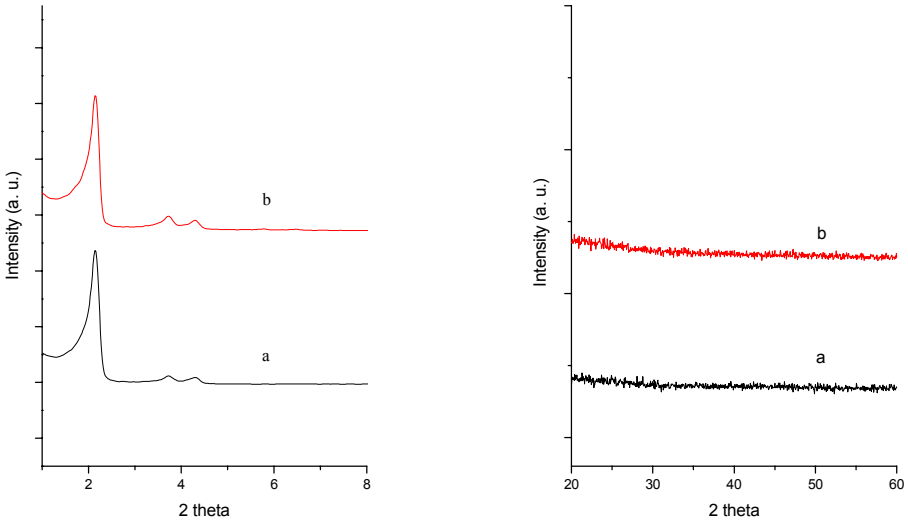


Figure S3: Powder XRD of Mn-MCM-41-as-synthesized (a) and Mn-MCM-41-vacuum at 350ºC (b).

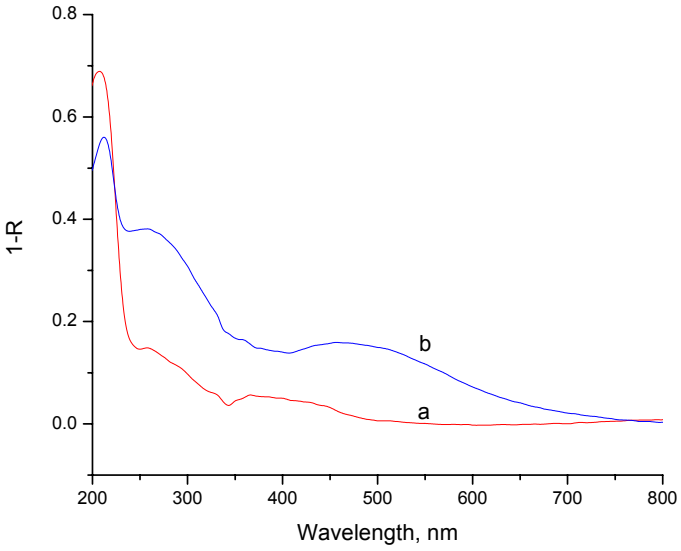


Figure S4: (a) DRS of $(Et_4N)_2MnCl_4$ (wt 2%) mixed with MCM-41.

(b) DRS of Mn-MCM-41 grafted using $(Et_4N)_2MnCl_4$ as precursor.

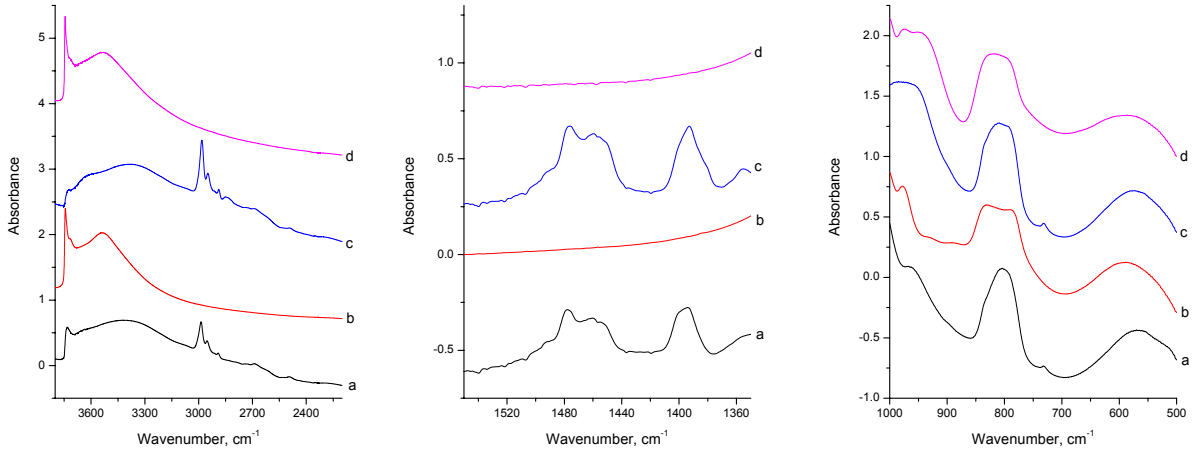
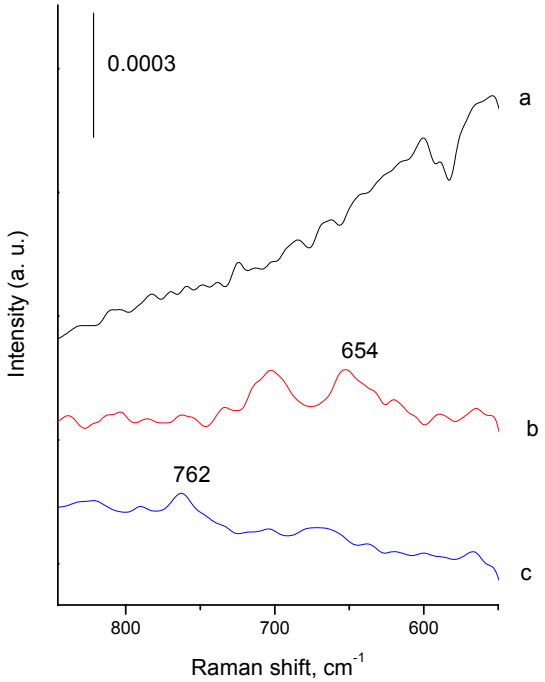
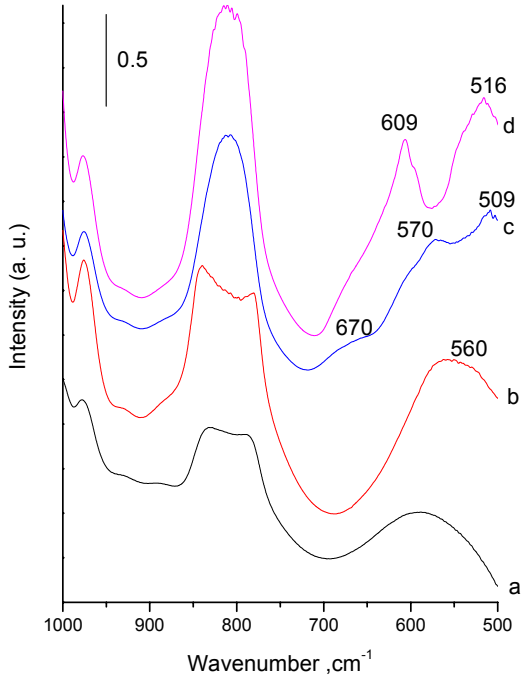


Figure S5: FTIR difference spectra of a) Mn-MCM-41-as-synthesized; b) Mn-MCM-41 heated under vacuum at 350 ºC; and c) TiMn-MCM-41-as-synthesized; (d) TiMn-MCM-41 heated under vacuum at 350 ºC.

(A)



(B)



(C)

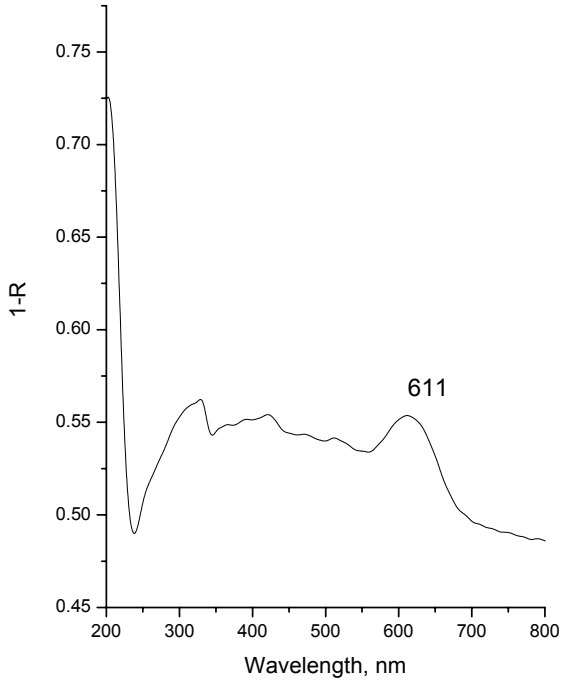


Figure S6: A. FT-Raman spectra of (a) Mn-MCM-41, (b) Mn_2O_3 (wt 2%) mechanically mixed with MCM-41, (c) MnO (wt 2%) mechanically mixed with MCM-41.

B. FT-IR spectra of (a) Mn-MCM-41, (b) MnO (wt 2%) mechanically mixed with MCM-41, (c) Mn_2O_3 (wt 2%) mechanically mixed with MCM-41, (d) Mn_3O_4 (wt 2%) mechanically mixed with MCM-41.

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

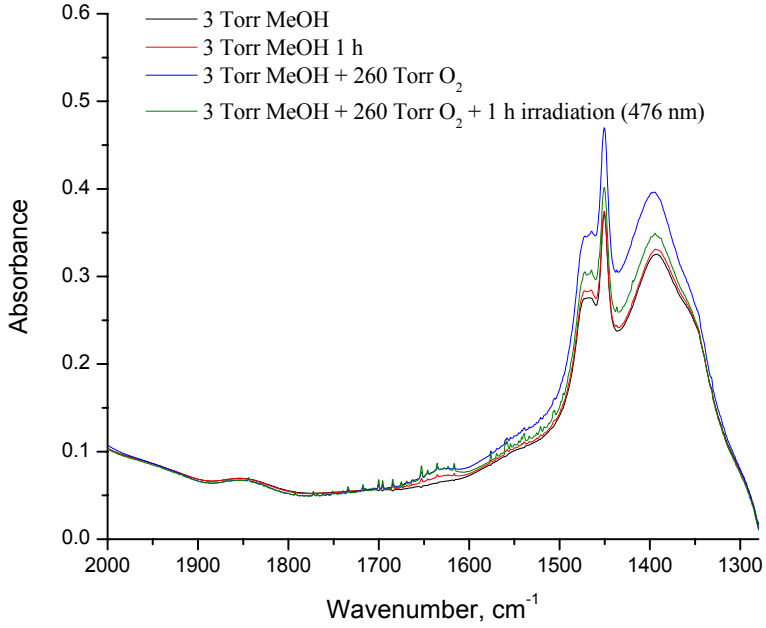


Figure S7: Infrared difference spectra of Ti-MCM-41 upon 3 Torr methanol loading, after 1 h waiting in the dark, after loading of 260 Torr O_2, and 476 nm irradiation for 1 h.