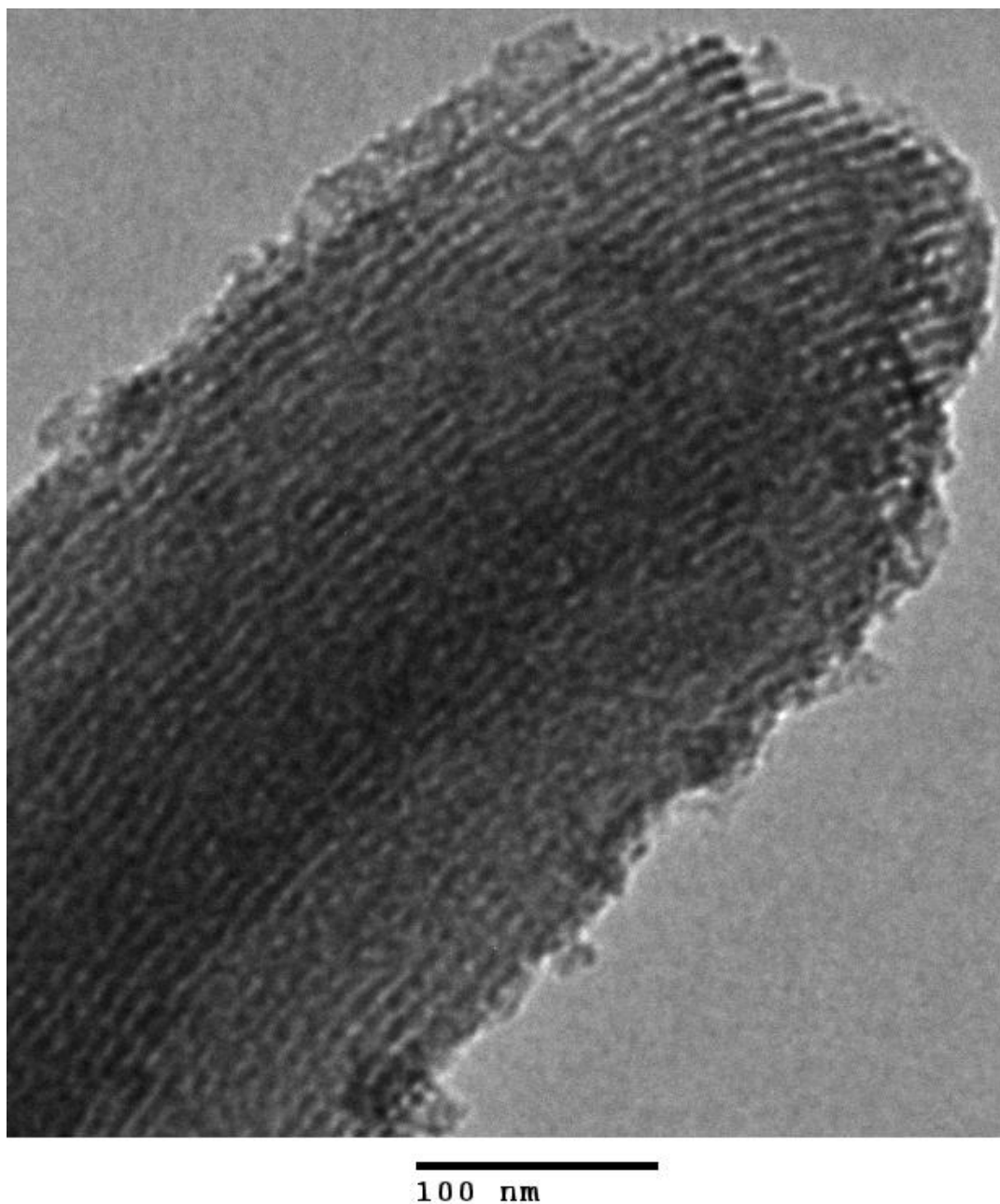


Supporting Information for:

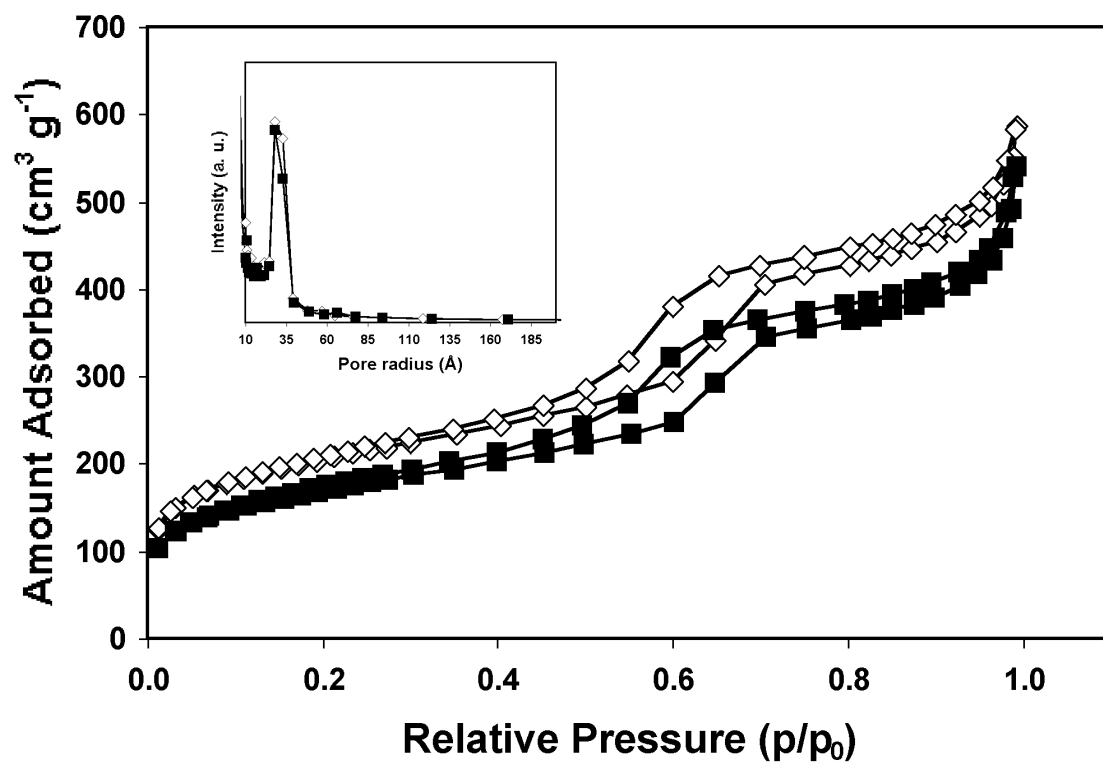
**Water Oxidation Catalysis by Immobilization of the Dimanganese Complex  $[\text{Mn}_2(\mu\text{-O})_2\text{Cl}(\mu\text{-O}_2\text{CCH}_3)(\text{bpy})_2(\text{H}_2\text{O})](\text{NO}_3)_2$  onto Silica.**

*Evan M. W. Rumberger, Hyun S. Ahn, Alexis T. Bell\*, and T. Don Tilley\**

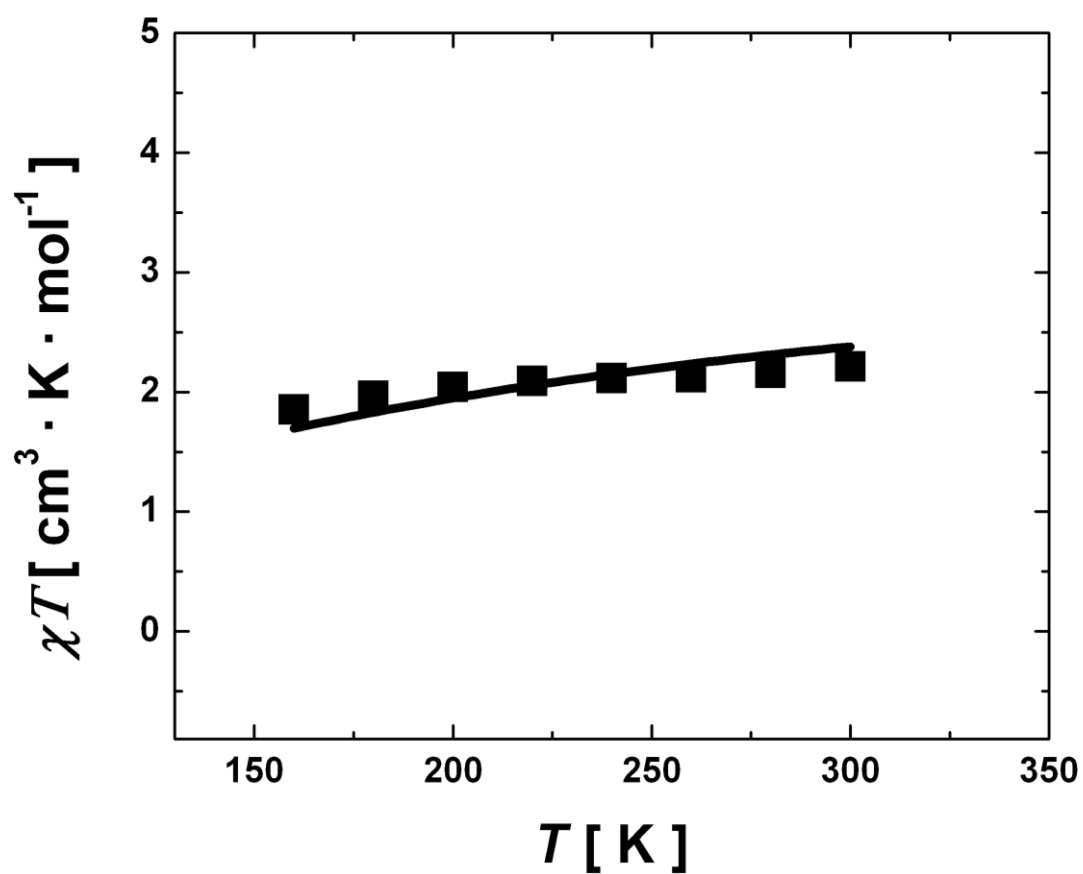
Departments of Chemistry and Chemical Engineering, University of California at Berkeley, Berkeley California 94720, and Chemical Sciences Division, Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, California 94720 USA



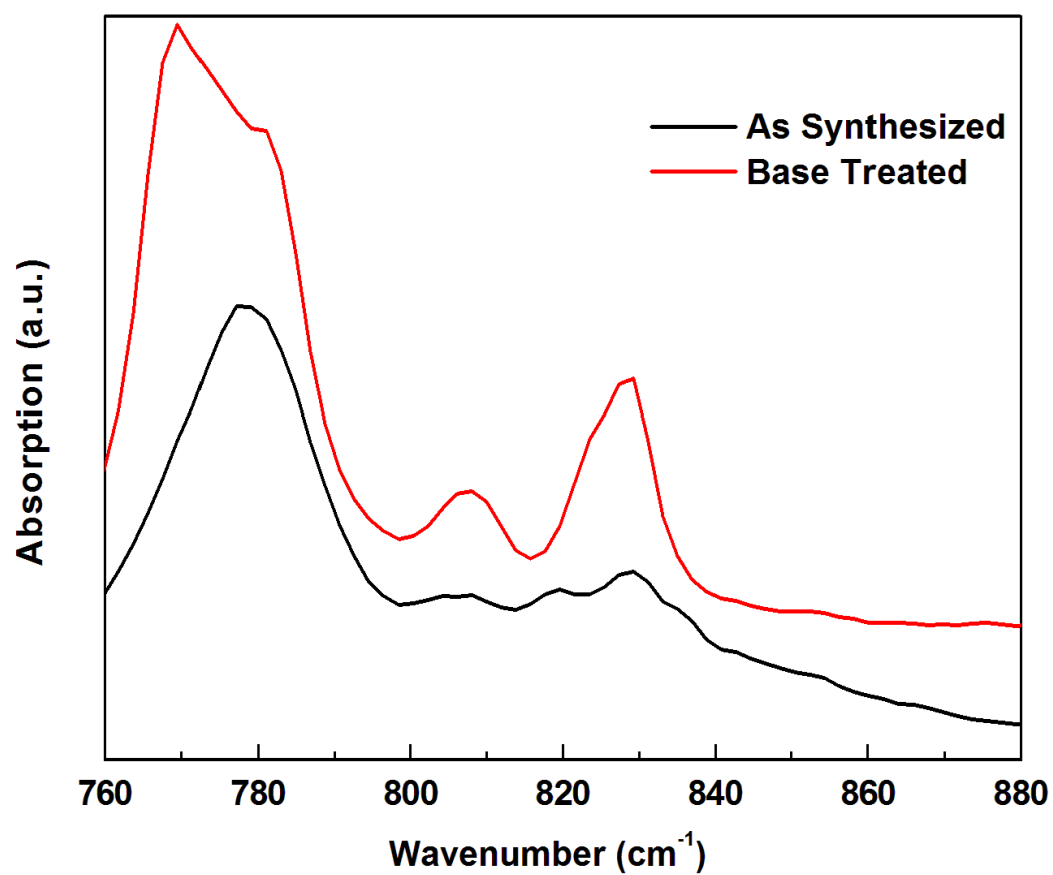
**Figure S1.** A typical TEM micrograph of the  $\text{Mn}_2\text{-SBA15(2)}$  material displaying no signs of Mn oxide nanoparticle formation (in the resolution of the instrument at ca. 10 nm).



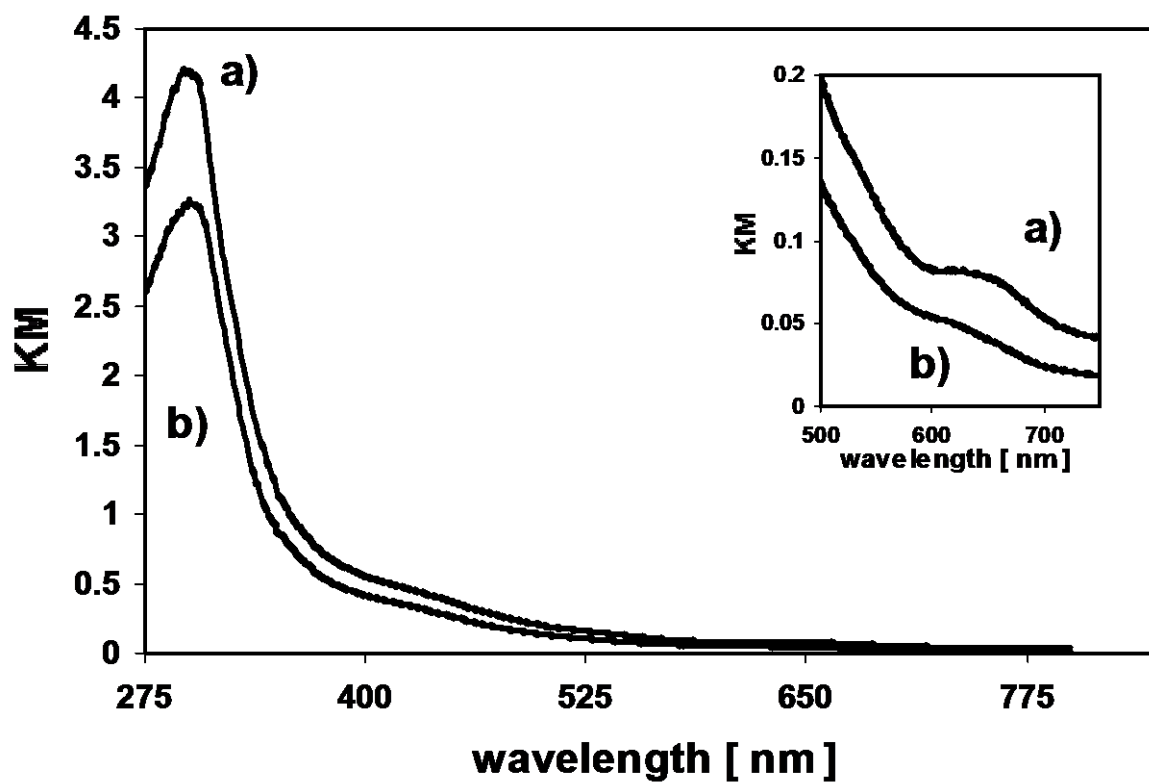
**Figure S2.** Nitrogen porosimetry adsorption / desorption isotherm with pore size distribution (insert) for the SBA15 ( $\diamond$ ) and  $\text{Mn}_2\text{-SBA15}$  ( $\blacksquare$ ) materials.



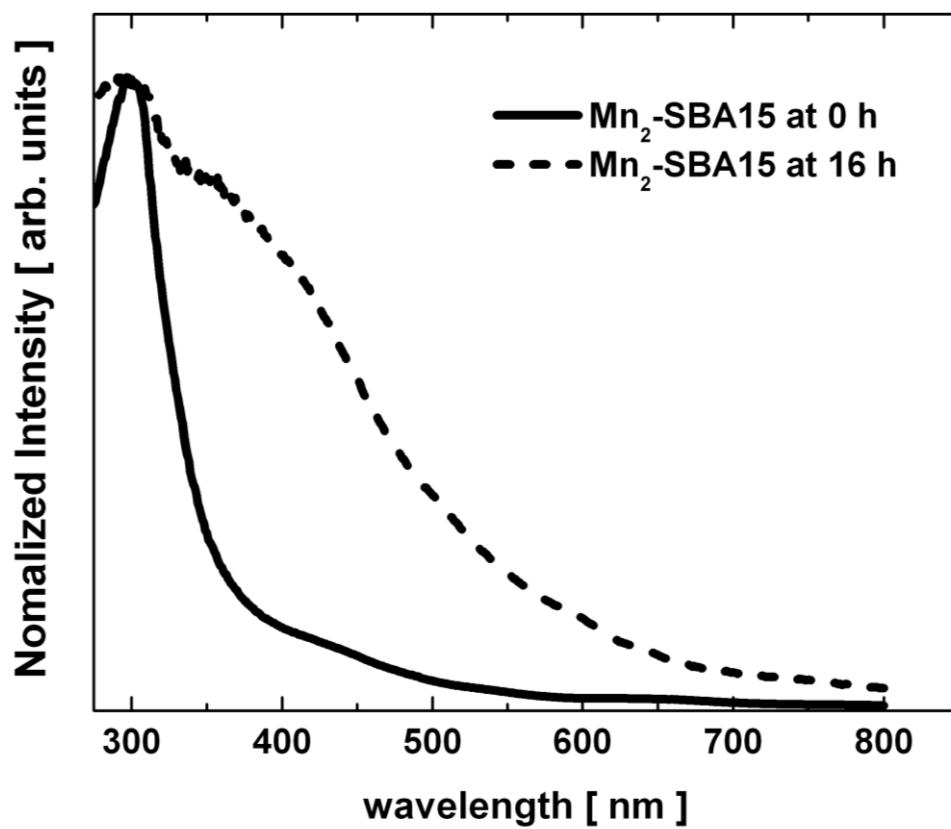
**Figure S3.** Plot of  $\chi T$  vs.  $T$  for the  $\text{Mn}_2\text{SBA15}$  (2) material where  $\chi$  is the molar susceptibility for the complex  $[\text{Mn}_2\text{O}_2\text{Cl}(\text{O}_2\text{CCH}_3)(\text{bpy})(\text{H}_2\text{O})]^{2+}$  grafted on to the SBA15. The solid line represents a least-squares fit to the data with  $g = 2.0$ ,  $J = -29 \text{ cm}^{-1}$ ; see the text for details.



**Figure S4.** Diffuse reflectance FTIR spectrum of as synthesized **1** and that of **1** after base treatment.



**Figure S5.** Diffuse reflectance UV-visible spectrum of the  $\text{Mn}_2\text{-SBA15}$  (**2**) material before (spectrum a) and after receiving a water treatment (b). The inset is a magnification of the 500 - 750 nm region.



**Figure S6.** Diffuse reflectance UV-visible spectrum of the Mn<sub>2</sub>-SBA15 (**2**) material before (solid line) and after being treated with a 200 mM solution of (NH<sub>4</sub>)<sub>2</sub>Ce(NO<sub>3</sub>)<sub>6</sub>.

**Table S1.** Parameters obtained from the analysis of the variable temperature magnetism data. Data for complex **1** are reproduced from reference 42.

	Complex <b>1</b>	Mn <sub>2</sub> SBA15 ( <b>2</b> )
g	1.97	2
J	-36.6 cm <sup>-1</sup>	-29 cm <sup>-1</sup>
χT @ 300K	2.23 cm <sup>3</sup> K mol <sup>-1</sup>	2.2 cm <sup>3</sup> K mol <sup>-1</sup>



**Magnetic properties of supported  $[\text{Mn}_2(\mu\text{-O})_2\text{Cl}(\mu\text{-O}_2\text{CCH}_3)(\text{H}_2\text{O})(\text{bpy})_2]^{2+}$ .** The data for  $\chi_{\text{MT}}$  versus temperature were least squares-fit to a theoretical model in order to ascertain the magnitude of the magnetic exchange interaction. The exchange interactions were represented with an isotropic spin Hamiltonian (eq. 1).

$$\hat{H} = -2J(\hat{S}_1\hat{S}_2) \quad (1)$$

Since

$$S_1 = S_2 \quad (2)$$

for the  $\text{Mn}^{\text{IV}}_2$  dinuclear complex **1**, there are only four possible total spin-states ( $S_T = 3, 2, 1, 0$ ). The eigenvalues of eq 2 were calculated using eq 3.

$$E(S_T) = -2S_T(S_T + 1) \quad (3)$$

Theoretical susceptibilities were calculated from a least-squares fit of the experimental data to the Van Vleck equation (eq 5). The results of the analysis are listed in Table 1.

$$\chi_M = \frac{Ng^2\beta^2}{3kT} \frac{\sum [S_T(S_T + 1)(2S_T + 1)]e^{-E(S_T)/k_B T}}{\sum (2S_T + 1)e^{-E(S_T)/k_B T}} \quad (5)$$