## SUPPLEMENTARY INFORMATION

## High Capacity CO<sub>2</sub> Adsorption in a Mg(II)-Based Phosphine Oxide Coordination Material

## Alisha M. Bohnsack,<sup>a</sup> Ilich A. Ibarra,<sup>a</sup> Peter W. Hatfield,<sup>b</sup> Young Kyu Hwang,<sup>c</sup> Ji Woong Yoon,<sup>c</sup> Jong-San Chang,<sup>c</sup> and Simon M. Humphrey<sup>a</sup>

<sup>a</sup> Department of Chemistry and Biochemistry, The University of Texas at Austin, 1 University Station A5300, Austin, TX 78712-0165, U.S.A. Tel: 1-(512)-471-0312; E-mail: smh@cm.utexas.edu

<sup>b</sup> University Chemical Laboratory, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, U.K.

<sup>c</sup> Catalysis Center for Molecular Engineering, Korea Research Institute of Chemical Technology, PO Box 107, Yusung, Daejeon, 305-600, Korea.



Figure S1. Solid-state MAS-<sup>31</sup>P-NMR spectrum for as-synthesized PCM-11.



Figure S2a. FT-IR spectrum of as-synthesized PCM-11 in KBr



**Figure S2b.** *In situ* temperature-dependent FT-IR spectra of as-synthesized PCM-11 upon heating under an inert atmosphere; loss of H<sub>2</sub>O from the pores appears complete above 100 °C in agreement with TGA data.



Figure S3. Comparative XRPD spectra for bulk samples of PCM-11 under various treatment conditions.



**Figure S4a.** Adsorption/desorption isotherms for as-synthesized PCM-11 after outgassing for 5 h at 200 °C, for: N<sub>2</sub> (black squares; 77 K); Ar (red circles; 87 K); O<sub>2</sub> (blue triangles; 77 K).



**Figure S4b.** Corresponding H<sub>2</sub> adsorption/desorption isotherm for as-synthesized PCM-11 under identical pretreatment conditions at 77 K.



**Figure S5a.** N<sub>2</sub> adsorption/desorption isotherms for CHCl<sub>3</sub> solvent-exchanged PCM-11 after outgassing for 5 h at 150 °C and after subsequent outgassing steps at higher temperature.



**Figure S5b.** H<sub>2</sub> adsorption/desorption isotherm for CHCl<sub>3</sub> solvent-exchanged PCM-11 after outgassing for 5 h at 200 °C.



Figure S6. The inferior high-pressure uptake of  $CO_2$  depicted by the adsorption/desorption isotherm for the the CHCl<sub>3</sub>-exhanged PCM-11 sample.