Supporting Information

Polymeric Organo-Magnesium Complex for Room Temperature Hydrogen Physisorption

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Hydrogen adsorption measurement:

Hydrogen adsorption measurements were performed by following the standard practice guidelines provided by the US Department of Energy to minimize potential errors in the hydrogen uptake measurement. The instrument calibration and the experimental considerations are described as follows. [1-3]

(1) Calibration:

- Calibration of volume, temperature sensors, pressure transducers
- Null calibration (empty sample chamber with zero uptake baseline under isothermal condition) (**Figure S1**)
- Calibration of the instrument with known materials (**Figure S2 and Figure S3**)

(2) Temperature monitoring and control:

- The temperature of the sample chamber was controlled to an acceptable level by applying water bath or liquid N_2 bath.
- The gas reservoir was thermostatted to minimize the room temperature fluctuations.

(3) Sample temperature was monitored continuously throughout the measurement.

(4) Adsorption equilibrium:

- Equilibrium was reached relatively quickly in the physisorption system and the pressure relaxation was measured at each step (data point was taken every minute).

(5) Sample size:

- Sample size was taken carefully to match up with the requirement on the system volume and the pressure measurement.
- Generally, sample size was taken to fill 2/3 volume of the sample chamber (3 cc).

(6) Gas purity: 99.9995 %

(7) Sample degassing was performed under ultra-high vacuum (UHV).

(8) Sample pretreatment: 150 ^{0}C under UHV for 12 h.

(9) Leakage was tested using helium and hydrogen at the maximum measurement pressure.

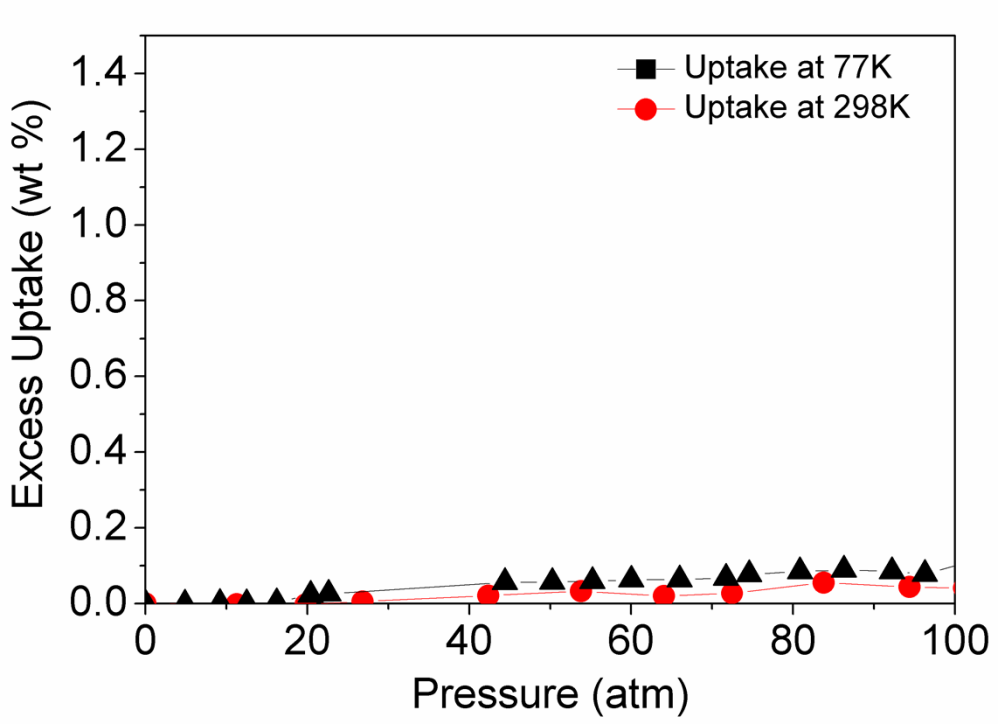

Figure S1: Empty sample holder calibration.

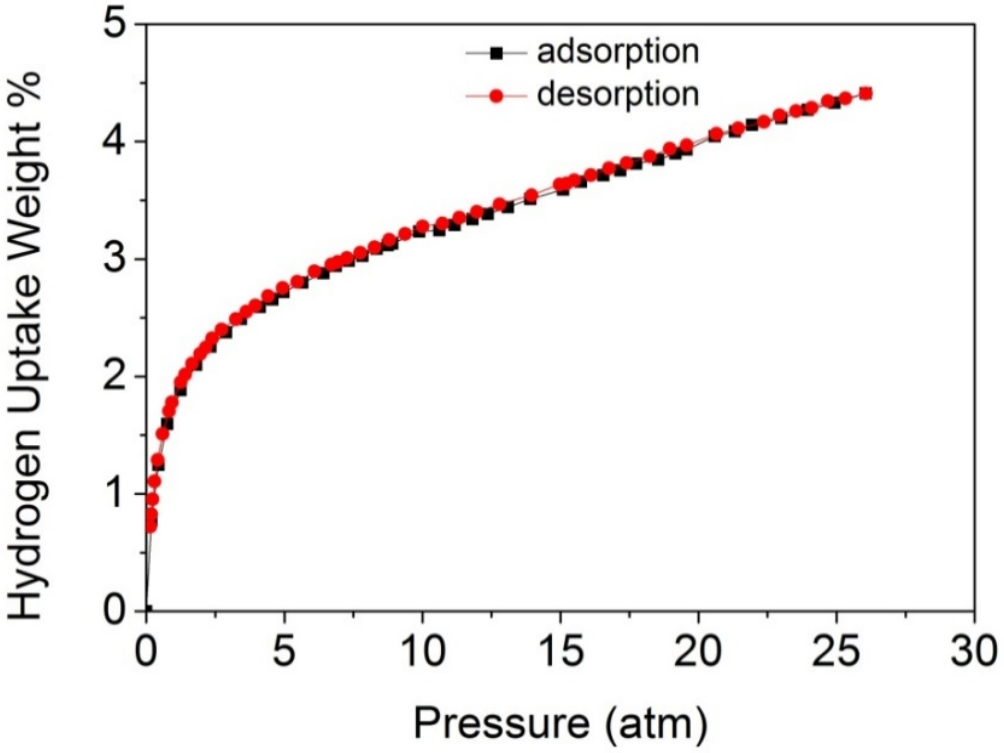

Figure S2: The total hydrogen storage capacity of commercially available basolite A100 MOF obtained at 77K in the same instrument under the similar conditions as the MTF-Mg material in this study, in agreement with the reported results in Reference. [4]

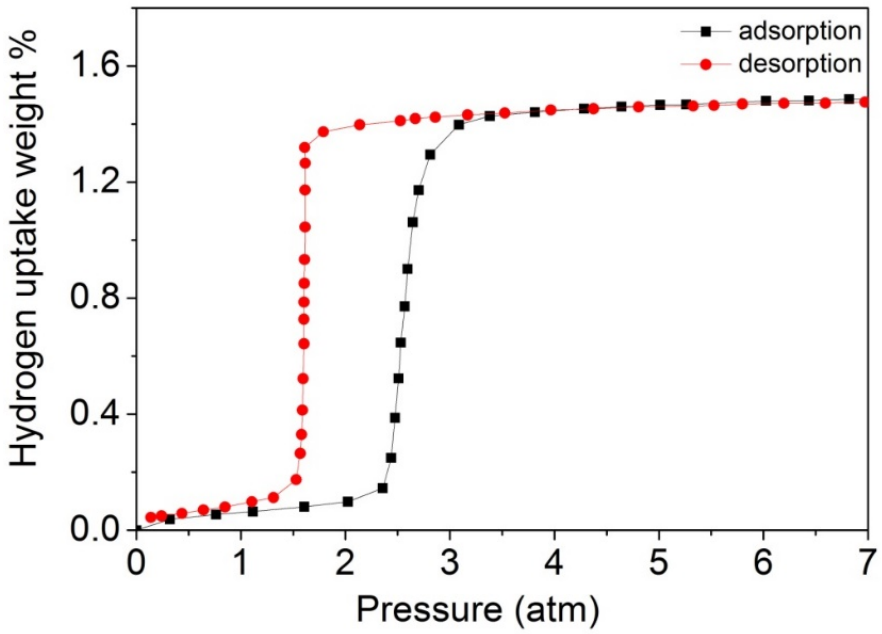

Figure S3: Hydrogen storage capacity of a commercially available $LaNi_5$ alloy obtained at 298K with the same instrument under the similar condition to the one hydrogen storage in the MTF-Mg material was measured. The results are in excellent agreement with the data shown in Reference. [5, 6]

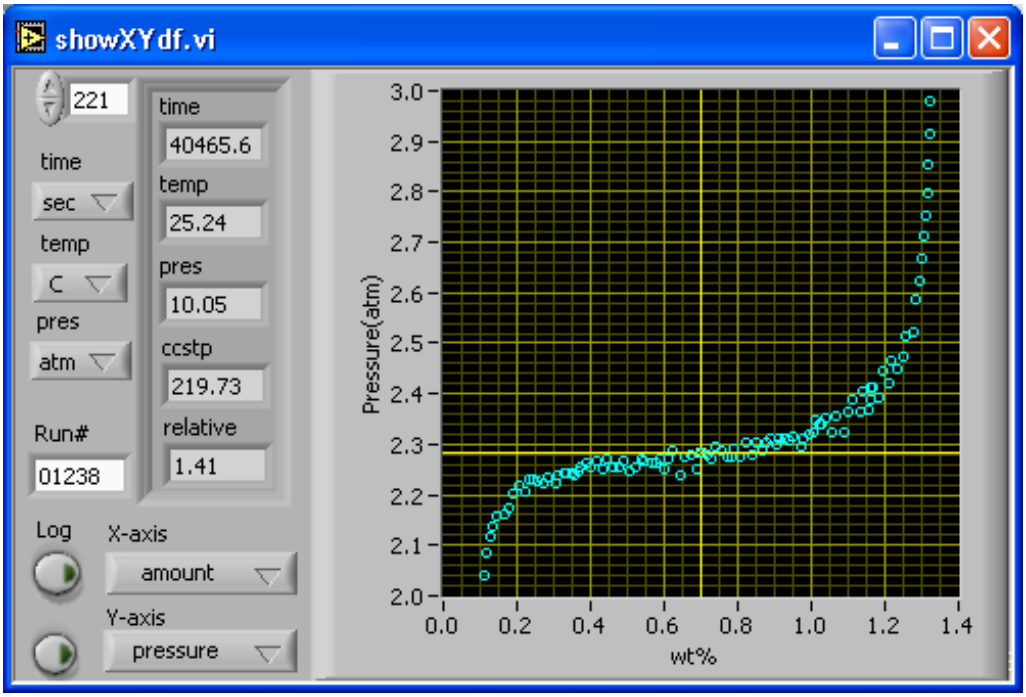

Figure S4: The pressure resolution of the instrument is 0.02 atm (LaNi5 at 298K)

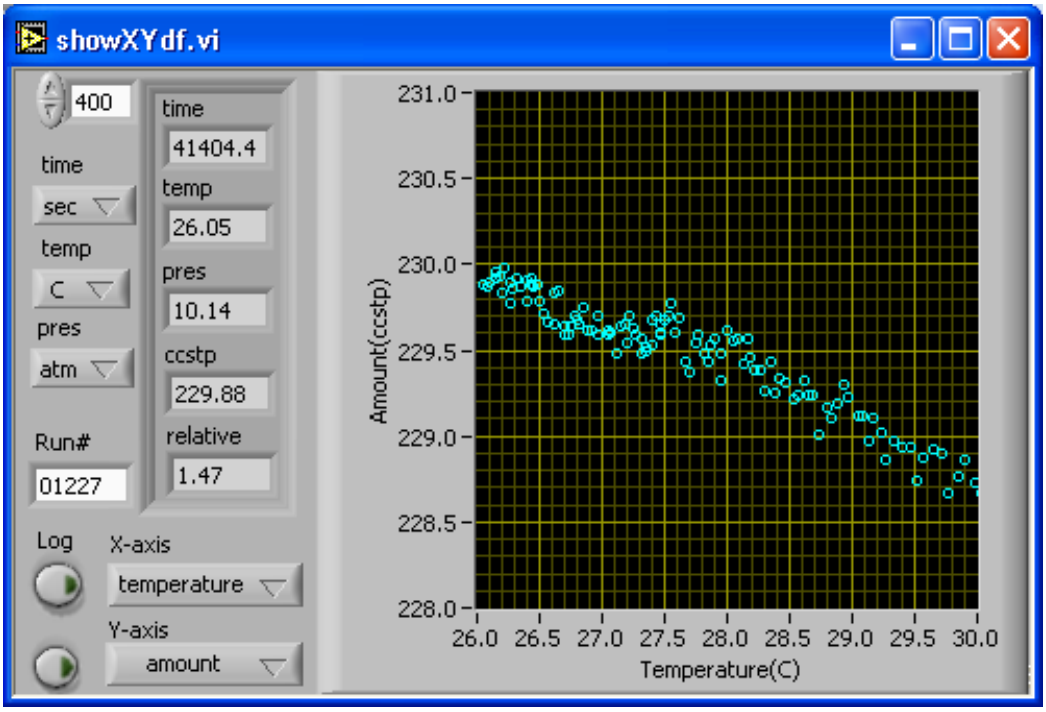

Figure S5: The gas measurement resolution with the GRC instrument is 0.2 ccstp.

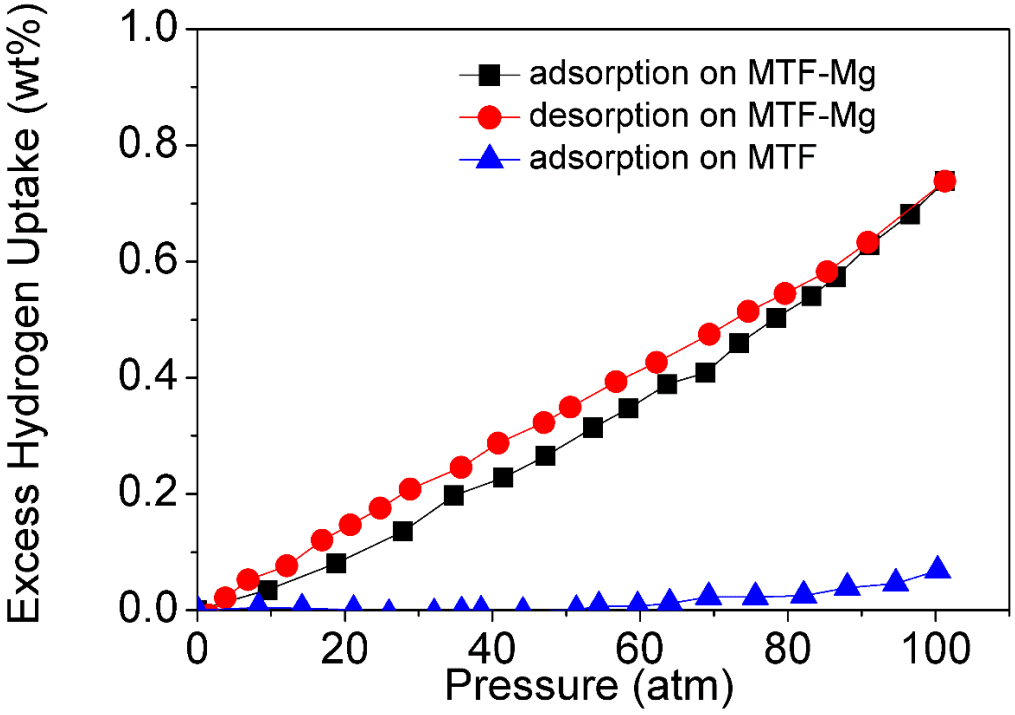

Figure S6: Excess hydrogen uptake at 298K and 100 atm in MTF-Mg and MTF.

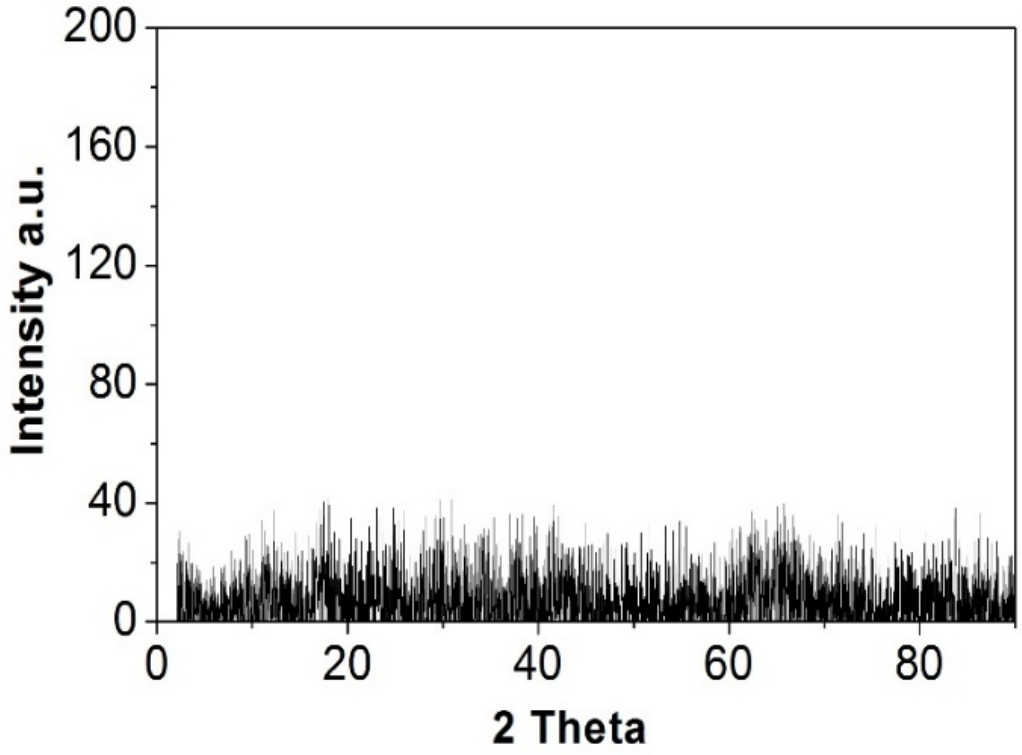

Figure S7: PXRD pattern of the MTF-Mg complex.

The powder X-ray diffraction profile of the MTF-Mg complex does not contain any sharp signals, which confirms that the material is amorphous with absence of long-range order.

References:

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2. D. P. M. Broom, P., *J. Alloys Compd.*, 2007, **446–447**, 687-691.
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4. G. Ferey, M. Latroche, C. Serre, F. Millange, T. Loiseau and A. Percheron-Guegan, *Chem. Commun.*, 2003, **0**, 2976-2977.
5. R. C. Bowman Jr, C. H. Luo, C. C. Ahn, C. K. Witham and B. Fultz, *J. Alloys Compd.*, 1995, **217**, 185-192.
6. S. Luo, J. D. Clewley, T. B. Flanagan, R. C. Bowman Jr and L. A. Wade, *J. Alloys Compd.*, 1998, **267**, 171-181.