Supporting Information

Polymer Framework with Continuous Pores for Hydrogen Getters: Molding and a Boost of Getter Rate

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1. Supplementary Experiments

Computed Tomography (CT): the specimen was cut to a small piece with size about 40 mm × 5 mm for micro-CT (computed tomography) testing. The high energy table scanner with the 225 kV micro-focus X-ray source and the detector plane with 2048 × 2048 sensors (size 200 μm) was used. The CT scan images of the specimen were obtained using the following settings: X-ray source 60 kV, 350 μA, magnification 11.89, 1.0 mm aluminum filter, frame-binning 4, CCD size 2048 × 2048, with 360 rotation steps over 360 degrees. The CT images were reconstructed using a cone-beam filtered back projection algorithm with isotropic voxels of size 13 μm.

Determination of DEB-Pd/C content in sheets:

A. *Sample processing:* All organics were burned and removed, and the DEB-Pd/C content was calculated by dimethylglyoxime gravimetry. Weighed about 1g of DEB-Pd/C powder (m_1, the same batch with raw material to prepare the sheet) with a ceramic crucible that had been burned with a constant weight, sintered at 600 ℃ for 2 hours in a muffle furnace. The residue was cooled down and transfered to a 400 mL beaker, dissolved with 10 mL aqua regia (3:1 concentrated hydrochloric acid and concentrated nitric acid), then concentrated to wet salt form, 10 mL concentrated hydrochloric acid was added, concentrated to wet salt form, the concentration step with concentrated hydrochloric acid was repeated twice.

B. *Gravimetric method*[1]： 10mL hydrochloric acid and 200mL water were added to solute the salt, 10mL of dimethylglyoxime solution (10 g L^{-1} in ethanol) was added dropwise while stirring, stirring was continued for 3min and still for 1h. Filter with suction to a 10 mL glass sand core crucible, the beaker and precipitate were washed 10 times with 2% hydrochloric acid solution, and 5 times with hot water at 85 °C. The crucible was baked at 110 °C for 1 hour, cooled and weighed (m_2).

Weighed about 2 g of sheet (m_1') in a ceramic crucible that had been burned with a constant weight, the precipitation weight m_2' was obtained as the same method described above.

The content of DEB-Pd/C was calculated by:

$$w\% = \frac{m_2'}{m_1'} \times \frac{m_1}{m_2} \times 100\% \quad (1)$$

C. *Inductively coupled plasma emission spectrometer (ICP) method*: Weighed about 1 g of sheet (or about 0.5 g powder) and processed by step A. The salt was dissolved and made up to volume with a volumetric flask by 1:20 hydrochloric acid. Experiments were taken out on Thermo iCAP 7400. Palladium standard solution (1000ug/ml in 2.0 mol/L hydrochloric acid, Aladdin, Shanghai, CN) was diluted into 5.00 ppm, 10.00 ppm, and 20.00 ppm as reference points in the working curve. 1:20 hydrochloric acid solution was used as a blank to determine the baseline.

[1] This method refers to the Chinese national standard: a) GB/T 23518-2009: Palladium on activated carbon catalyst. b) GB/T 15072.4-2008: Test method of precious metal alloys – determination of palladium content for palladium and silver alloys - butanedione dioxime gravimetry.

Determination of specific surface area: Determination of specific surface area was carried out on BET instrument (Autosorb iQ Station 2, Quantachrome Instruments, US), nitrogen was used as analysis gas. Nitrogen adsorption/desorption isotherms were determined at 77 K, then surface areas of all samples were calculated by the Brunauer-Emmett-Teller method.

2. Supplementary Figures

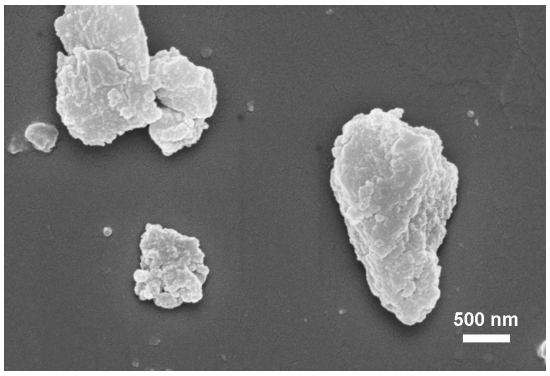

Figure S1. SEM image of DEB-Pd/C powder after ball-milling.

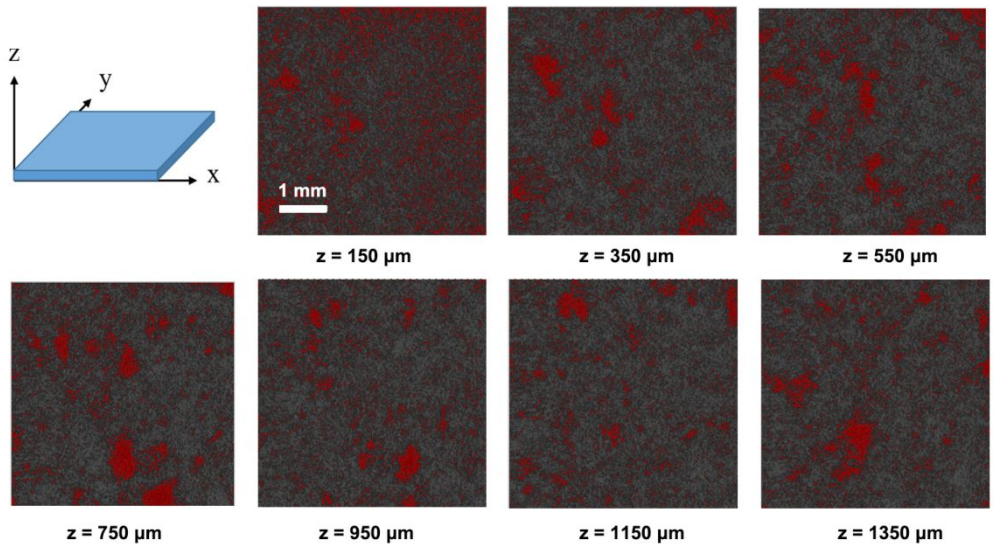

Figure S2. Computed tomography reconstruction imaging of a hydrogen getter sheet (25% DEB-Pd/C, 30% PEO: (PEO+LDPE) ratio) in different depth. Red dot represents pores.

3. An example of determination of DEB-Pd/C content in composite sheet.

Table S1. Content of DEB-Pd/C in sheets calculated by two methods

<table>
<tr><td>Method</td><td>Data*</td><td colspan="4">Content of DEB-Pd/C in sheets</td></tr>
<tr><td>Calculation through preparation</td><td>m_{LDPE}:45.5 g
m_{PEO}: 24.5 g
$m_{DEB\text{-}Pd/C}$: 30.0 g</td><td colspan="4">$w_{prep} = \frac{m_{DEB-Pd/C}}{m_{DEB-Pd/C} + m_{LDPE}} \times 100\% = 39.7\%$</td></tr>
<tr><td>Calculation by dimethylglyoxime precipitation method</td><td>Powder:
m_1: 1.4872 g
m_2: 0.1358 g
Sheet:
m_1': 2.0046 g
m_2': 0.0706 g</td><td colspan="4">Content of Pd in DEB-Pd/C powder (w_1):
$w_1 = \frac{m_2}{m_1} \times \frac{Mw_{Pd}}{Mw_{Pd-DGO2}} \times 100\% = 2.87\%$ **
Content of Pd in sheets (w_2):
$w_2 = \frac{m_2'}{m_1'} \times \frac{Mw_{Pd}}{Mw_{Pd-DGO2}} \times 100\% = 1.11\%$
Content of DEB-Pd/C in sheets:
$w = \frac{w_2}{w_1} = \frac{m_2'}{m_1'} \times \frac{m_1}{m_2} \times 100\% = 38.7\%$</td></tr>
<tr><td rowspan="9">Determined by ICP</td><td rowspan="9">m_{sheet} = 1.0026 g
m_{powder} = 0.4978</td><td></td><td>c_{Pd} (ppm)</td><td colspan="3">Intensity of Pd peaks (a. u.)</td></tr>
<tr><td></td><td></td><td>324.2 nm</td><td>340.4 nm</td><td>360.9 nm</td></tr>
<tr><td>blank</td><td>0</td><td>-6.177</td><td>4.112</td><td>-1.464</td></tr>
<tr><td>R1</td><td>5.00</td><td>2352.</td><td>5157.</td><td>3194.</td></tr>
<tr><td>R2</td><td>10.00</td><td>4791.</td><td>10490.</td><td>6534.</td></tr>
<tr><td>R3</td><td>20.00</td><td>9602.</td><td>20970.</td><td>13070.</td></tr>
<tr><td>Sheet</td><td>10.98</td><td>5253</td><td>11488</td><td>7174</td></tr>
<tr><td>Powder</td><td>14.25</td><td>6819</td><td>14908</td><td>9311</td></tr>
<tr><td colspan="4">$w_{Pd-sheet} = \frac{c_{Pd-sheet} \times m_{powder}}{m_{sheet} \times c_{Pd-powder}} \times 100\% = 38.26\%$</td></tr>
</table>

*The methods are based on the same sheet with 30% DEB-Pd/C weight fraction and with 35% PEO:(LDPE+PEO) ratio in preparation.

** Pd-DGO2: Palladium dimethylglyoxime.

4. BET results and discussion

Surface area of DEB-Pd/C powder: 83.697 $m^2\ g^{-1}$

Surface area of DEB-Pd/C-LDPE sheet: 6.816 $m^2\ g^{-1}$

Surface area of compact sheet: 0.012 m^2 g^{-1}

The specific surface area of the Pd/C catalyst was close to 1000 m^2 g^{-1}, and the specific surface area was greatly reduced after being ball-milled with DEB into Pd/C-DEB hydrogen absorber powder. And after molding with HDPE, the specific surface area further decreased, which was still much larger than the compact sheet without pore-creating process.