

# Supporting Information

## (Pt-C<sub>60</sub>)@SiO<sub>2</sub> Nanocomposites for Convenient Chemical Hydrogen Storage

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### Experimental Section

All chemicals were purchased from Sigma–Aldrich.

#### **Synthesis of monodisperse iron–platinum (FePt) nanocrystals:**

K<sub>2</sub>PtCl<sub>4</sub> (3×10<sup>-4</sup> mol), FeCl<sub>3</sub> (3×10<sup>-4</sup> mol), and sodium dodecyl sulfate (SDS, 3×10<sup>-4</sup> mol) were well dispersed in a flask containing deionized water (75 mL), and the solution was refluxed at 70 °C. Hydrazine (N<sub>2</sub>H<sub>4</sub>; 1 mL) was added drop by drop to the above solution. After reaction for 12 h, the black product was precipitated by adding ethanol (20 mL) and isolated after centrifugation and dried under N<sub>2</sub> for 24 h.

#### **Synthesis of FePt-C<sub>60</sub> nanocomposites:**

The C<sub>60</sub> (200 mg) and polyvinyl pyrrolidone (PVP, 0.5 g, MW≈50000) were well dissolved in toluene solution (20 mL), and then the solution was given ultrasonic treatment for 5 h at room temperature. The above solution was added drop by drop to the as-prepared FePt nanocrystals dispersed in aqueous solution (20 mL). The resulting mixture was constant magnetic stirring at room temperature for 12 h, then the obtained samples were washed with ethanol and dried under N<sub>2</sub> for 24 h.

#### **Synthesis of (FePt-C<sub>60</sub>)@SiO<sub>2</sub> nanocomposites:**

TEOS (4.5 mL) was rapidly added into a mixture containing cetyltrimethylammonium bromide (CTAB, 0.18 g), ethanol (100 mL), H<sub>2</sub>O (45 mL), ammonium hydroxide (15 mL) and FePt-C<sub>60</sub> nanocomposites dispersed in aqueous solution (20 mL). The resulting mixture was constant magnetic stirring at room temperature for 12 h, and then the obtained samples were washed with ethanol and dried under N<sub>2</sub> for 24 h.

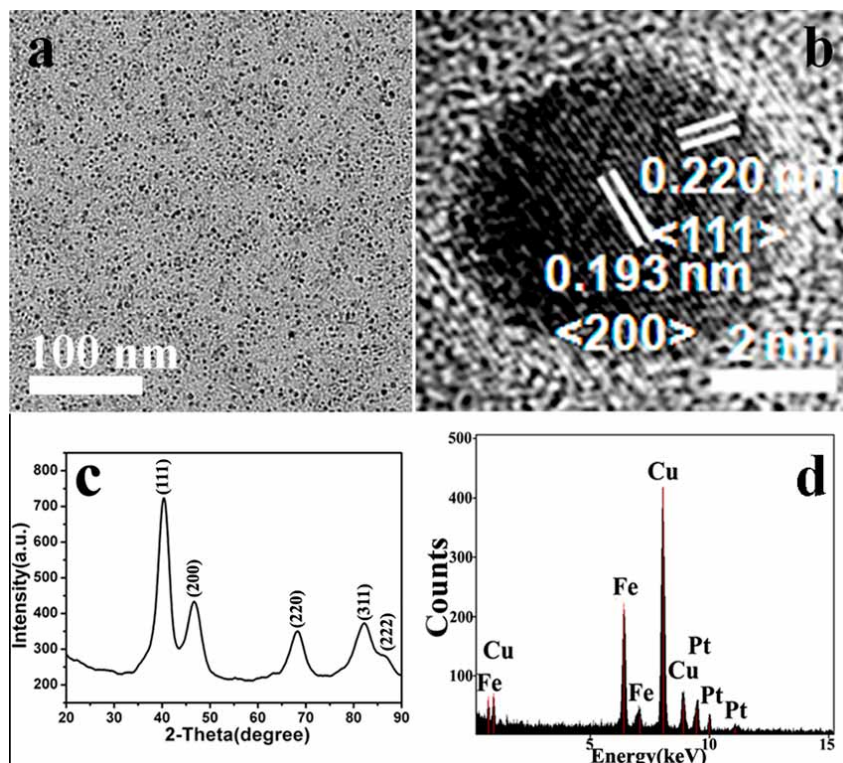
#### **Synthesis of (Pt-C<sub>60</sub>)@SiO<sub>2</sub> nanocomposites:**

The as-synthesized (FePt-C<sub>60</sub>)@SiO<sub>2</sub> nanocomposites (0.5 g) was added to HCl (2 M, 100 mL). The mixture was constant magnetic stirring at room temperature for 12 h, and then the obtained samples were washed with distilled water and dried under N<sub>2</sub> for 24 h.

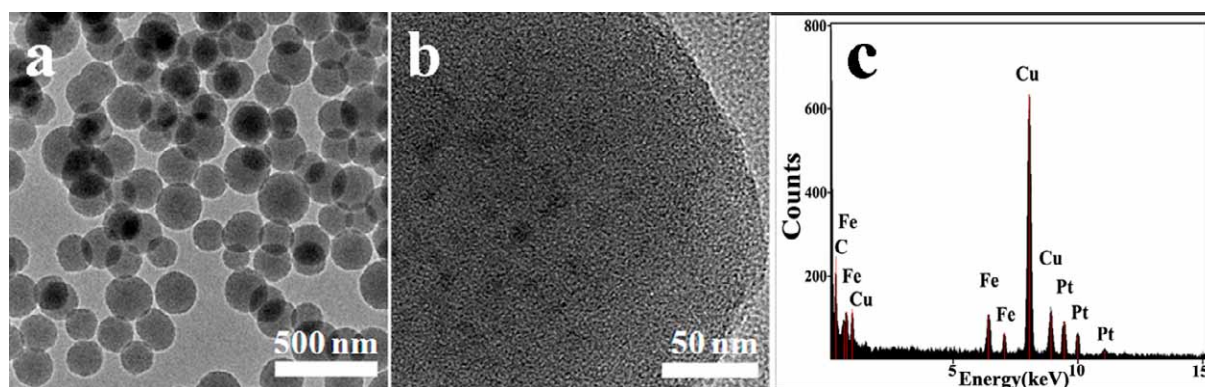
#### **Characterization:**

SEM images were taken on a FEI-quanta 200F scanning electron microscope with acceleration voltage of 20 kV. The TEM image and HRTEM images were obtained with a FEI/Philips Tecnai 12 BioTWIN transmission electron microscope operated at 200 kV with EDX analyses. The TEM samples were prepared by dropping the sample solution onto a copper grid covered with carbon and dried in air. The FT-IR spectra were obtained with a Nicolet 360 spectrometer. Raman spectra were collected on an HR 800 Raman spectroscope (J Y, France) equipped with a synapse CCD detector and a confocal Olympus microscope, the spectrograph uses 600 g mm<sup>-1</sup> gratings and a 514 nm He–Ne laser. The Thermogravimetric (TG) was carried out by Universal Analysis 2000 thermogravimetric analyzer in N<sub>2</sub> with a heating rate of 10 °C /min. BET specific surface areas and pore size distributions were calculated by plotting the adsorption isotherm of N<sub>2</sub> at liquid N<sub>2</sub> temperature (77 K). Hydrogen gas adsorption was carried out at room temperature and 1-10 bar. These measurements were made on a Micromeritics ASAP 2050 porosimeter. Hydrogen chemisorption test of (Pt-C<sub>60</sub>)@SiO<sub>2</sub> nanocomposites was carried out with ASAP analyzer (ASAP 2020) at 273 K. The chemical hydrogen adsorption measurements were also performed using a gravimetric method at 268 K and atmospheric pressure, while the desorption measurements were performed at 393 K and atmospheric pressure. By considering that the correct measurement of hydrogen adsorption is essential to achieving a proper evaluation of a given material, we have included a detailed description of the experimental procedure and the equipment used in this work. The gravimetric analysis of the hydrogen adsorption/desorption capacity for the product was measured by a magnetic suspension balance gravimetric analyzer (Rubotherm (Germany),

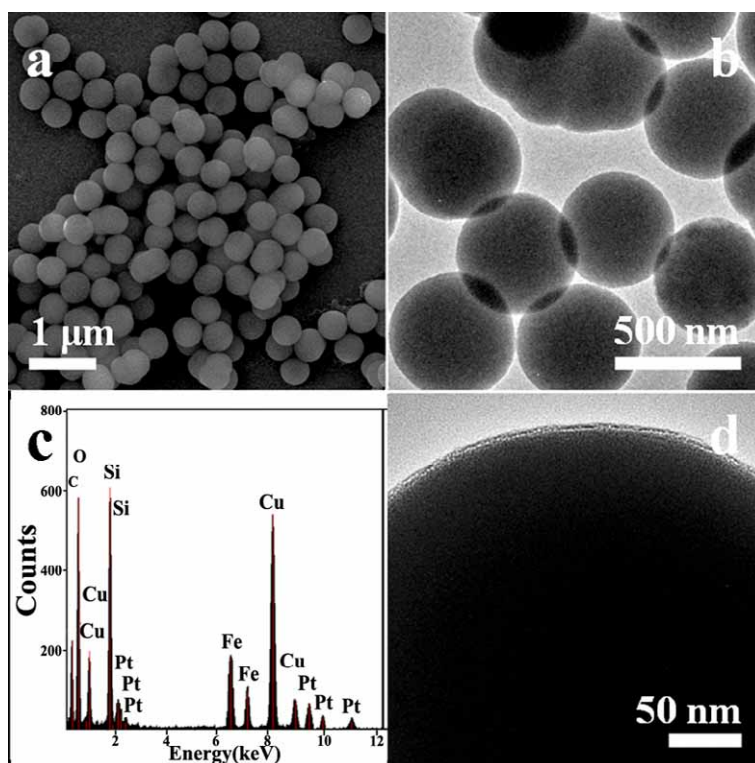
the sensitivity of the balance is 0.1 mg). The (Pt-C<sub>60</sub>)@SiO<sub>2</sub> nanocomposites were degassed at 573 K for 6 h before the measurements. The temperature of the flask was maintained at 268 K during the adsorption, while the desorption of temperature was kept at 393 K. Hydrogen is introduced up to the desired condition, and when thermodynamic equilibrium is reached, the value of the weight indicated by the balance is collected. The measured weight increase corresponds to the hydrogen adsorption. From this value, the amount of hydrogen adsorbed/desorbed is calculated using the weight of sample. Hydrogen chemisorption test of (Pt-C<sub>60</sub>)@SiO<sub>2</sub> nanocomposites was carried out with ASAP analyzer (ASAP 2020) at 273 K.



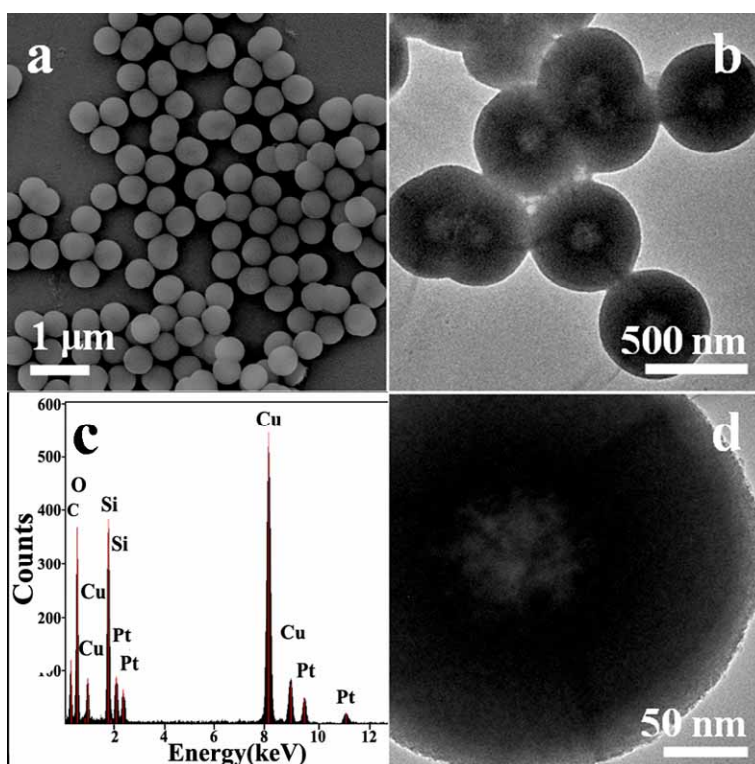
**Fig. S1.** Structural characterization of FePt nanocrystals: (a) TEM image, (b) HRTEM image, (c) XRD patterns, and (d) EDX spectrum..



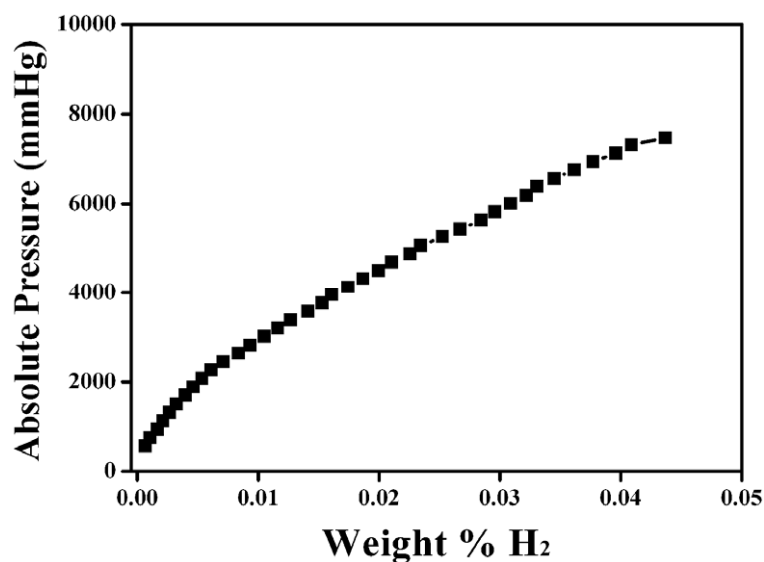
**Fig. S2.** Structural characterization of FePt-C<sub>60</sub> nanocomposites: (a) TEM image, (b) magnified TEM image, and (c) EDX spectrum.



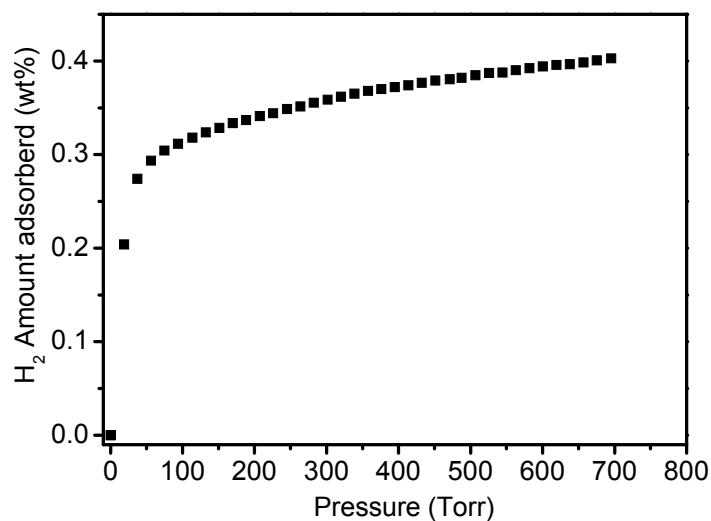
**Fig. S3.** Structural characterization of (FePt-C<sub>60</sub>)@SiO<sub>2</sub> nanocomposites: (a) SEM image, (b) TEM image, (c) EDX spectrum, and (d) magnified TEM image.



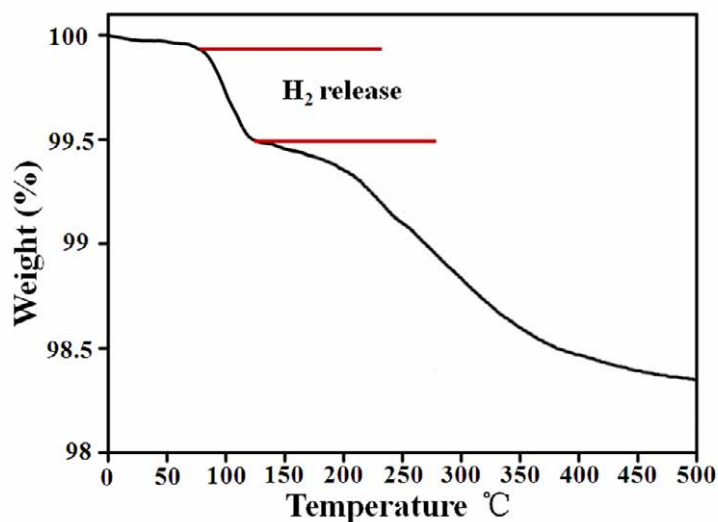
**Fig. S4.** Structural characterization of (Pt-C<sub>60</sub>)@SiO<sub>2</sub> nanocomposites: (a) SEM image, (b) TEM image, (c) EDX spectrum, and (d) magnified TEM image.



**Fig. S5.** Hydrogen gas adsorption isotherm of (Pt-C<sub>60</sub>)@SiO<sub>2</sub> nanocomposites at room temperature and 10 bar.



**Fig. S6.** Low-pressure isotherm of H<sub>2</sub> at 273 K on (Pt-C<sub>60</sub>)@SiO<sub>2</sub> nanocomposites.



**Fig.S7.** The TG profile for (Pt-C<sub>60</sub>)@SiO<sub>2</sub> nanocomposites after chemical hydrogen storage.