Supporting Information

Polypyrrole-coated flower-like Pd nanoparticles (Pd NPs@PPy) with enhanced stability and heat conversion efficiency for cancer photothermal therapy

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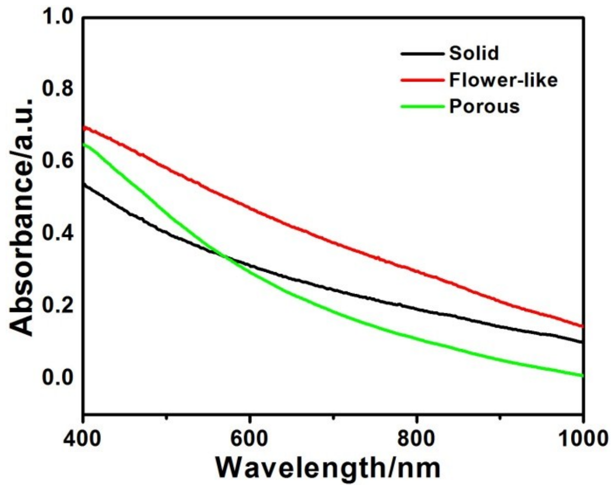

Fig. S1. UV−vis-NIR absorption spectra of solid, flower-like and porous Pd NPs at the concentration of 30.0 μg mL^{-1}.

Preparation of the solid and porous Pd NPs：

The solid and porous Pd NPs were prepared through a seed-mediated. The preparation of seed solutions was the same to the flower-like Pd NPs. For the growth of the Pd NPs, 0.025 mL seed solution was added to a mixture solution made of 9.70 mL CTAC (4.5 mM) and 0.30 mL H_2PdCl_4 (0.01 M). After tuning the pH of the solution to 4 (to obtain solid Pd) and 8 (to obtain porous Pd NPs), respectively, 0.1 mL ascorbic acid (0.1M) was added to the above mixture solution under magnetic stirring. After mixed for 15 s, the mixture solution was left undisturbed at room temperature for 5 h.

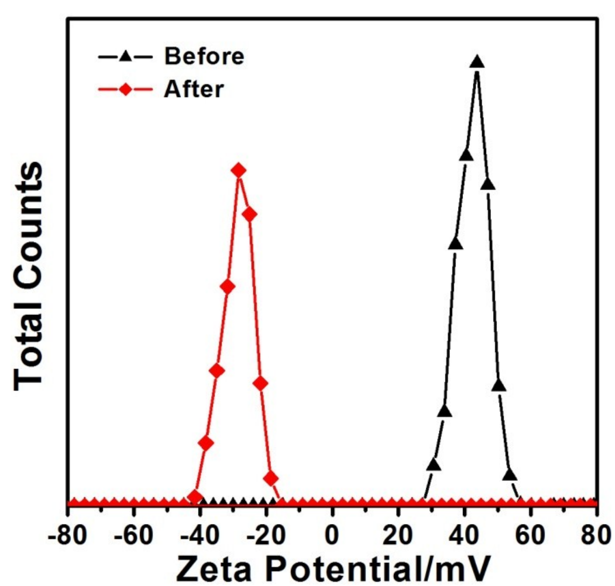

Fig. S2. ξ potential distribution of the Pd NPs before and after ligand exchange.

Table S1. Comparison of the molar extinction coefficient of flower-like Pd NPs and Pd NPs@PPy with different PPy thickness.

PPy thickness/nm	0	2	4	7	12
A_{808}	0.3694	0.4106	0.4646	0.4921	0.5652
$\varepsilon_{808}/M^{-1}\cdot cm^{-1}$	1.67×10^{11}	1.85×10^{11}	2.10×10^{11}	2.22×10^{11}	2.55×10^{11}

Calculation of the photothermal transduction efficiency.

According to the method reported by Roper, the energy transfer obeys the following relation:

$$Q = Q_{NPs} + Q_{Dis} - Q_{surr} = \sum_i m_i C_{p,i} \frac{dT}{dt}$$

Where Q is the energy required for the system, Q_{NPs} and Q_{Dis} represent the heat generated by NPs and quartz cell under laser irradiation, Q_{surr} is the heat conduction away by air, m and C_p are the mass and heat capacity of water, respectively.

The laser-induced source term, Q_{NPs}, represent heat dissipated by electron-phonon relaxation of the plasmon on the Pd NPs suface for 808 nm irradiation:

$$Q_{NPs} = I(1-10^{-A_{808}})\eta$$

Where I is incident laser power, A_{808} is the absorption intensity at 808 nm, η stands for photothermal transduction efficiency.

In addition, Q_{surr} is in proportion to the temperature variation between system and environment, which is expressed as:

$$Q_{surr} = hS(T - T_{surr})$$

Where *h* is heat transfer coefficient, *S* is the surface area of the container, and T_{surr} is the ambient temperature.

When the system is heated to a maximum value in temperature (T_{max}) where the heat input is equal to heat output:

$$Q_{NPs} + Q_{Dis} = Q_{output} = hs(T_{\max} - T_{surr})$$

$$I(1-10^{A_{808}})\eta + Q_{Dis} = hs(T_{\max} - T_{surr})$$

Then the η can be calculated according to:

$$\eta = \frac{hS(T_{\max} - T_{surr}) - Q_{Dis}}{I(1-10^{A_{808}})}$$

Where Q_{Dis} is measured independently to be 61 mW. However *hS* remains unknown. In order to get the *hS*, the cooling stage is studied. The system gives out energy with a decrease in temperature:

$$Q_{output} = -\sum_i m_i C_{p,i} \frac{dT}{dt} = hS(T - T_{surr})$$

We replace:

$$\tau_s = \frac{\sum_i m_i C_{p,i}}{hs}$$

And θ is introduced using the maximum system temperature, T_{max}.

$$\theta = \frac{T - T_{surr}}{T_{\max} - T_{surr}}$$

$$\frac{d\theta}{dt} = \frac{1}{\tau_s}[\frac{Q_{NPs} + Q_{Dis}}{hS(T_{\max} - T_{surr})} - \theta]$$

$$\frac{d\theta}{dt} = \frac{-\theta}{\tau_s}$$

$$t = -\tau_s \ln\theta + b$$

Take PPy@Pd as the example, the time constant for heat trasfer from system is determined to be 356.3 by applying the linear time data from the cooling period (after 25 min) *vs* negative natural logarithm of driving force temperature. In addition, the m_{water} and m_{quartz} is 2 g and 5.831 g, C_{water} and C_{quartz} is 4.2 J g^{-1} K^{-1} and 0.892 J g^{-1} K^{-1}, respectively. Thus, the η of PPy@Pd is 96.0%, and the η of the Pd NPs@PPy with different PPy thicknesses are listed in Table S2.

Table S2. Comparison of the photothermal conversion efficiency of the Pd NPs@PPy with different PPy thickness.

PPy thickness/nm	0	2	4	7	12
η/%	90.9	92.6	93.8	96.0	87.4