Supporting Information

PdAu-based nanotheranostic agent for photothermal initiation and oxygen-independent free radicals generation

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Calculation of the Photothermal Conversion Efficiency

The photothermal conversion efficiency $\eta$ of APPG nanocomposites was calculated according to the reported method\cite{1}. The detailed calculation was using the following eq 1:

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

(1)

where $h$ is heat transfer coefficient, $S$ is the surface area of the container, $T_{\text{max}}$ is the equilibrium temperature, $T_{\text{surr}}$ is the ambient temperature of the surroundings. $Q_{\text{Diss}}$ is heat losted from light absorbed of the container itself, which was measured independently containing pure water without AIPH-PAPG. And $A_{808}$ is the absorption intensity of AIPH-PAPG at 808 nm. The value of $hS$ is derived according to eq. 2:

$$\tau_s = \frac{m_D C_D}{hS}$$

(2)

where $\tau_s$ is the sample system time constant, $m_D$ and $C_D$ are the mass and heat capacity of ultrapure water used as the solvent, respectively.

And, $\tau_s$ can be calculated by eq. 3:

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

(3)

Time constant for heat transfer from the system is determined to be $\tau_s = 314.7$ s applying to the linear time data from the cooling period (after 600 s) vs the negative natural logarithm of driving force temperature (Fig. 3c). Substituting the value of $\tau_s$ into eq 2, $hS$ can be obtained. And the value of $hS$ replaced into eq. 1, 808 nm photothermal conversion efficiency $\eta$ of APPG nanocomposites can be calculated to be 24.6%.
Fig. S1 XRD pattern of PdAu alloy nanoparticles and the corresponding standard cards of Au (JCPDS 89-3697) and Pd (JCPDS 46-1043).
**Fig. S2** TEM image of Gd-BSA complexes. (Inset: HRTEM image of Gd-BSA complexes)
Fig. S3 Photothermal curves of APPG nanocomposites aqueous dispersion (400 μg·mL⁻¹) under varied power densities (0.5, 0.7, 1.0, and 1.5 W·cm⁻²).
Reference