Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

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

Feng Wang,[ab] Zaoxia Sun,[c] Zhuo Wang,[d] Junxun Zhou,[e] and Lining Sun*[ab]

[a] Department of Chemistry, College of Sciences, Shanghai University, Shanghai 200444, P.R. China. E-mail: lnsun@shu.edu.cn

[b] Research Center of Nano Science and Technology, College of Sciences, Shanghai University, Shanghai 200444, P.R. China.

[c] Institute of Nanochemistry and Nanobiology, Shanghai University, Shanghai 200444, P.R. China.

[d] State Key Laboratory of Marine Resource Utilization in South China Sea, Special Glass Key Lab of Hainan Province, Hainan University, Haikou 570228, P.R. China.

[e] Department of Pharmacy, School of Medicine, Shanghai University, Shanghai 200444, P.R. China.

Calculation of the Photothermal Conversion Efficiency

The photothermal conversion efficiency η of APPG nanocomposites was calculated according to the reported method[1]. The detailed calculation was using the following eq 1:

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

where h is heat transfer coefficient, S is the surface area of the container, T_{max} is the equilibrium temperature, T_{surr} is the ambient temperature of the surroundings. Q_{Dis} 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:

$$\tau_s = \frac{m_D C_D}{hS} \quad (2)$$

where τ_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, τ_s can be calculated by eq. 3:

$$t = -\tau_s ln\theta \quad (3)$$

Time constant for heat transfer from the system is determined to be τ_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 τ_s into eq 2, hS can be obtained. And the value of hS replaced into eq. 1, 808 nm photothermal conversion efficiency η of APPG nanocomposites can be calculated to be 24.6%.

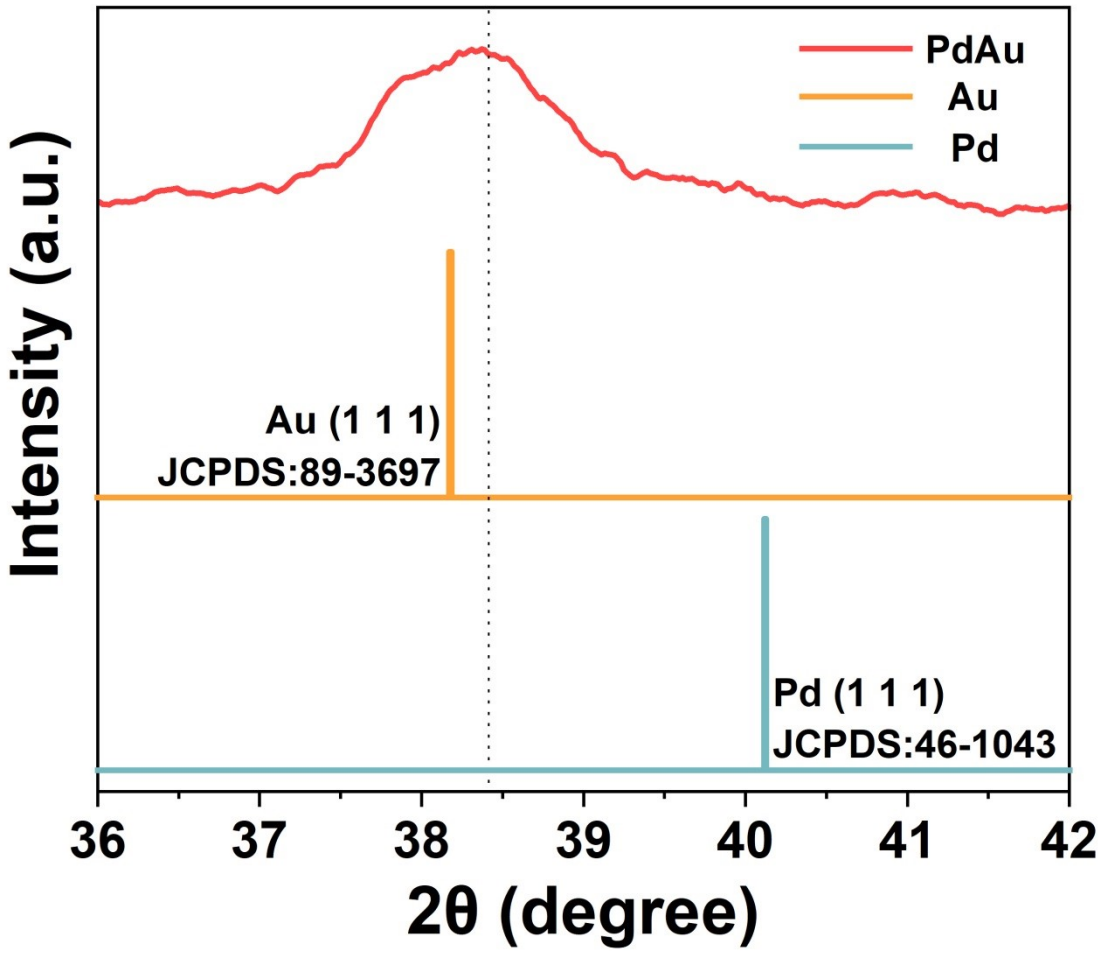

Fig. S1 XRD pattern of PdAu alloy nanoparticles and the corresponding standard cards of Au (JCPDS 89-3697) and Pd (JCPDS 46-1043).

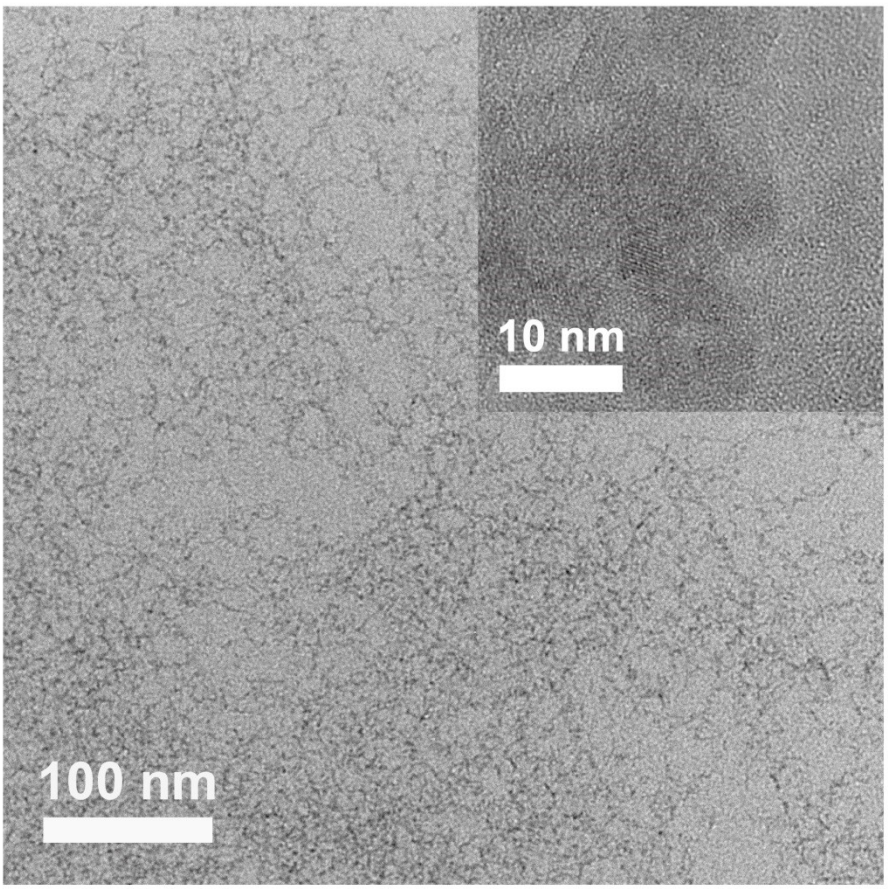

Fig. S2 TEM image of Gd-BSA complexes. (Inset: HRTEM image of Gd-BSA complexes)

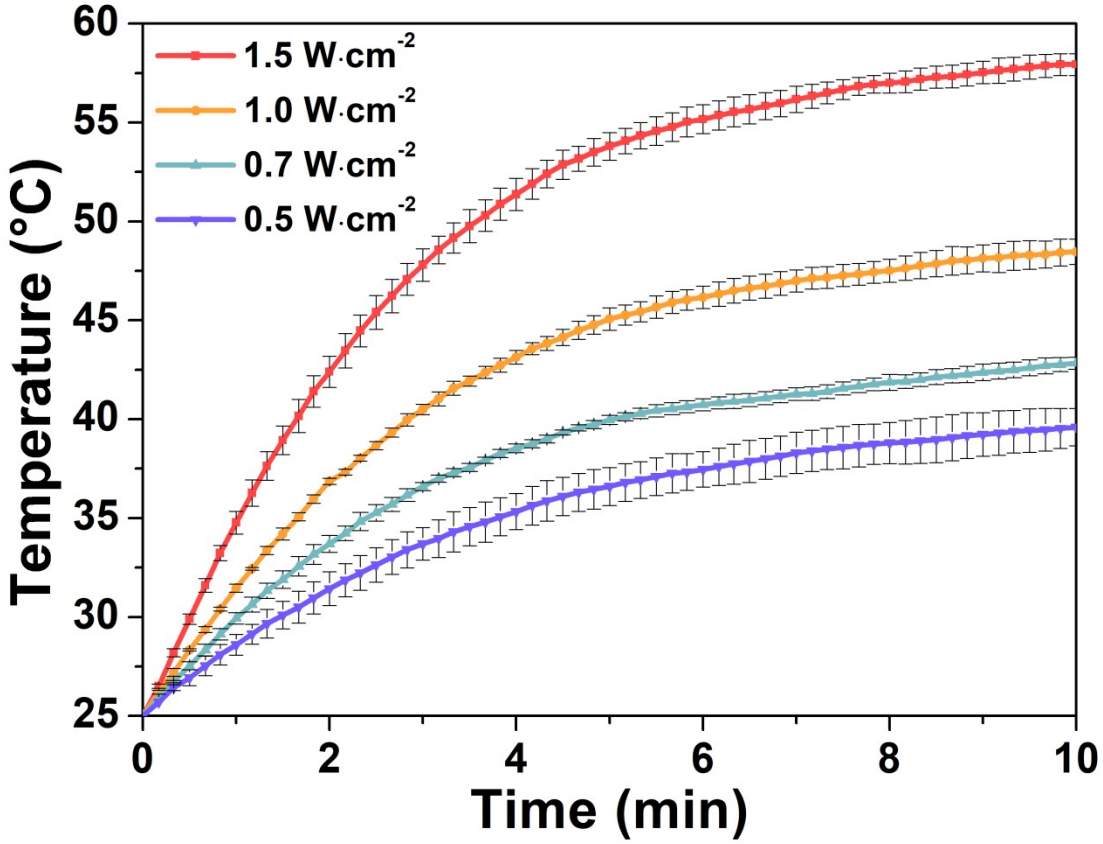

Fig. S3 Photothermal curves of APPG nanocomposites aqueous dispersion (400 μg·mL^{-1}) under varied power densities (0.5, 0.7, 1.0, and 1.5 W·cm^{-2}).

Reference

[1] D. K. Roper, W. Ahn and M. Hoepfner, *J. Phys. Chem. C*, 2007, **111**, 3636-3641.