Electronic Supplementary Material (ESI) for New Journal of Chemistry. This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2022

Supplementary Information

Preparation of gold@europium-based coordination polymer nanocomposite structures with excellent photothermal properties and its four-mode imaging technique

Faming Xia, a Xuejiao Gao, Xiaomei Shen, Hualan Xub*, Shengliang Zhong*

^a Key Lab of Fluorine and Silicon for Energy Materials and Chemistry of

Ministry of Education, College of Chemistry and Chemical Engineering,

Jiangxi Normal University, Nanchang, 330022, China

^bAnalytical and Testing Center, Jiangxi Normal University, Nanchang 330022,

China

*corresponding author.

*E-mail: slzhong@jxnu.edu.cn

Calculation of the photothermal conversion efficiency

Following literature report¹, the total energy balance for the system is

$$\sum_{i} m_i C_{p,i} \frac{dT}{dt} = Q_{NPS} + Q_S - Q_{loss}$$
(1)

where *m* and *Cp* are the mass and heat capacity, respectively. The suffix "*i*" of *m* and *Cp* refers to solvent(water) or dispersed matter (nanoprods). *T* is the solution temperature. Q_{NRs} is the photothermal energy absorbed by GNRs@EuCP NPs per second:

$$Q_{NRs} = I (1 - 10^{-A_{980}}) \eta$$
 (2)

where *I* is the laser power, $A\lambda$ is the absorbance of GNRs@EuCP at the wavelength of 980 nm in aqueous solution, and η is the photothermal conversion efficiency of GNRs@EuCP NRs which means the ratio of absorbed light energy converting to thermal energy.

 $Q_{\rm loss}$ is thermal energy lost to the surroundings:

$$Q_{loss} = hA\Delta T \tag{3}$$

Where *h* is the heat transfer coefficient, *A* is the surface area of the container, and ΔT is the changed temperature, which is referred to T-T_{surr} (T and T_{surr} are the solution temperature and ambient temperature of the surrounding, respectively).

*Q*s is the heat associated with the light absorbed by solvent per second. In the situation of heating pure water, the heat input is equal to the heat output at the maximum steady-statue temperature, so the equation can be:

$$Q_S = Q_{loss} = hA\Delta T_{max,H_2O} \tag{4}$$

Where $\Delta T_{\text{max,H2O}}$ is the temperature change of water at the maximum steady-state temperature. As it to the experiment of GNRs@EuCP NRs dispersion, the heat inputs are the heat generated by Nanoparticles (QNRs) and the heat generated by water (Qs), which is equal to the heat out put at the maximum steady-statue temperature, so the equation can be:

$$Q_{NPs} + Q_s = Q_{loss} = hA\Delta T_{max,mix}$$
(5)

Where $\Delta T_{\max,\min}$ is the temperature change of the GNRs@EuCP NRs dispersion at the maximum steady state temperature. According to the equation (2), (4) and (5), the photothermal conversion efficiency (η) can be expressed as following:

$$\eta = \frac{hA\Delta T_{max,mix} - hA\Delta T_{max,H_20}}{I(1 - 10^{-A_{980}})} = \frac{hA(\Delta T_{max,mix} - \Delta T_{max,H_20})}{I(1 - 10^{-A_{980}})}$$
(6)

In this equation, only hA is unknown. In order to get the hA, we introduce θ , which is defined as the ratio of ΔT to ΔT_{max} :

$$\theta = \frac{\Delta T}{\Delta T_{max}} \tag{7}$$

Substituting equation (7) into equation (1):

$$\frac{d\theta}{dt} = \frac{hA}{\sum_{i} m_{i}C_{p,i}} \left[\frac{Q_{NPs} + Q_{s}}{hA\Delta T_{max}} - \theta\right]$$
(8)

When the laser was shut off, the $Q_{\text{NPs}} + Q_{\text{s}} = 0$, equation (8) could be expressed to:

$$dt = -\frac{\sum_{i}^{i} m_{i} C_{p,i}}{hA \quad \theta} \tag{9}$$

Equation (9) changes the expression:

$$t = -\frac{\sum_{i}^{i} m_{i}C_{p,i}}{hA} ln\theta$$

$$\underbrace{\sum_{i}^{i} m_{i}C_{p,i}}_{I}$$
(10)

Where hA can be calculated by linear relationship of time versus $-\ln(\theta)$. As the m_{H₂0} was 2 g. Cp_{,H₂0} was 4.2 J⁻¹g⁻¹. So we can get hA equals 0.0295.

According to equation (6), ΔT max,mix was 50°C. ΔT max,_{H₂0} is 12°C. *I* was 1.57 W where the area of light spot was 3.14 cm². A₉₈₀ was 1.365 Thus, the photothermal conversion efficiency (η) of GNRs@EuCP NRs could be calculated to be 74.6%.

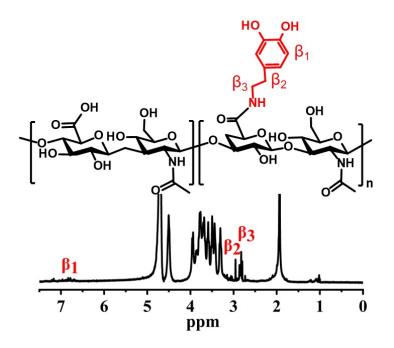


Fig. S1 1HNMR spectra of HA1.

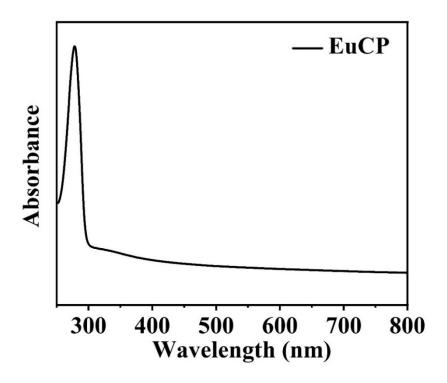


Fig. S2 UV-vis-NIR spectra of EuCP.

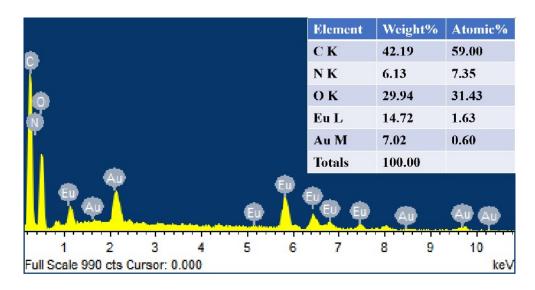


Fig. S3 EDS spectra of GNRs@EuCP.

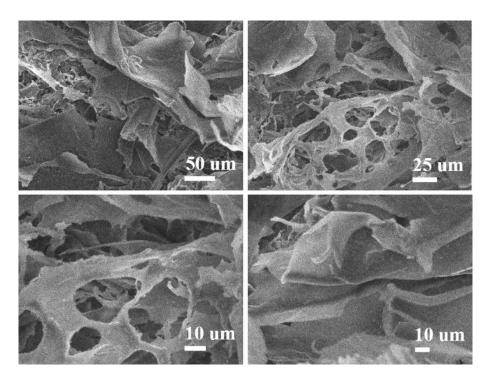


Fig. S4 SEM images of EuCP.

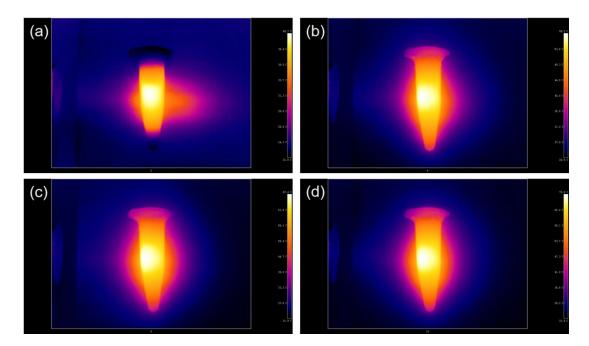


Fig. S5 (a, b, c, d). Corresponding infrared thermal images of GNRs@EuCP at 2, 6, 8 and 10 min intervals.

References

 W. Ren, Y. Yan, L. Zeng, Z. Shi, A. Gong, P. Schaaf, D. Wang, J. Zhao, B. Zou, H. Yu, G. Chen, E. M. Brown and A. Wu, *Adv. Healthc. Mater.*, 2015, 4, 1526-1536.