Supporting Information

Fine-Tuning LSPR Response of Gold Nanorod/Polyaniline Core-Shell Nanoparticles with High Photothermal Efficiency for Cancer Cell Ablation

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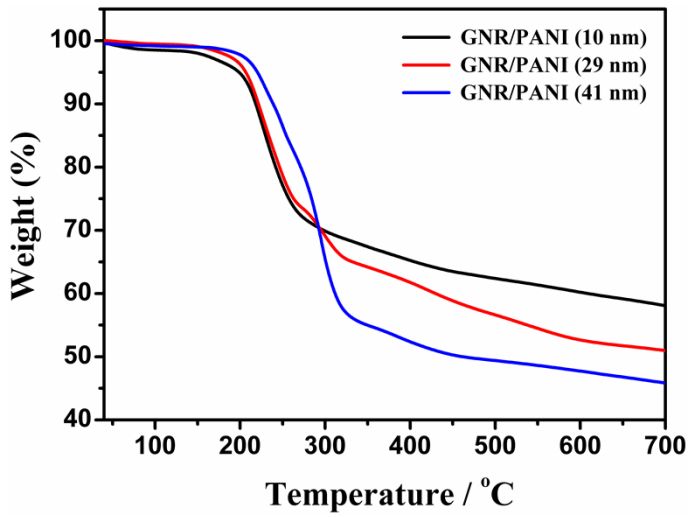

Figure S1. TGA curves of three GNR/PANI samples with different PANI shell thickness.

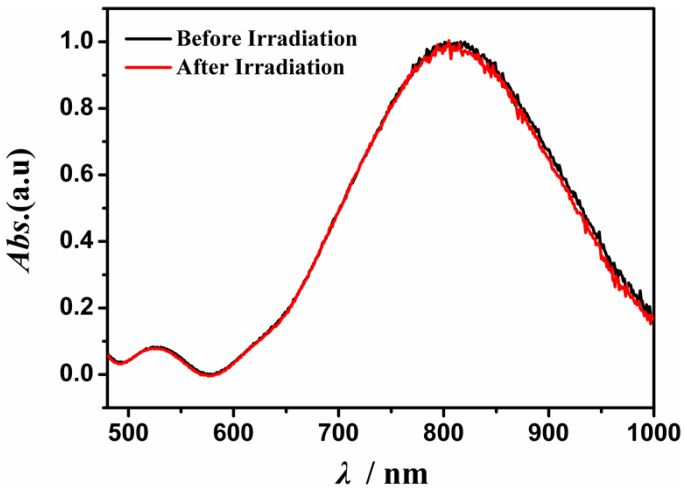

Figure S2. UV-vis-NIR spectra of GNR/PANI nanoparticles before and after laser irradiation at the power density of 1.8 W cm^{-2} for 1 h.

Photothermal Conversion Efficiency Calculations:

The Q_{abs} and Q_{tot} can be calculated by the equations as below:

$$Q_{tot} = (\text{laser power}) \times (\text{laser beam spot}) \times (\text{irradiation time}) \quad (1)$$

$$Q_{abs} = [(M_{Au} \times Cp_{Au}) + (M_{P\text{-unit}} \times Cp_{P\text{-unit}}) + (M_{w} \times Cp_{W})] \times (\Delta T) \quad (2)$$

where the laser beam spot is 0.2 cm^2, the irradiation time is 10 mins, the laser powers were different for various power density. For equation (2), M_{Au}, $M_{P\text{-unit}}$, M_{w}, Cp_{Au}, $Cp_{P\text{-unit}}$, Cp_{W} and ΔT represent moles of Au in the nanomaterial, moles of PANI repeat unit in the nanomaterial, moles of water, heat capacity of Au, heat capacity of PANI repeat unit, heat capacity of water and change in temperature after 10 min irradiation, respectively. As shown Figure S1, the dopant anions, moisture and PANI content is approximately 50 wt% of the GNR/PANI sample with PANI shell thickness of 29 nm. Based on the concentration of the rest Au content (50 wt%, 18 mg kg^{-1}), the PANI content concentration can be calculated as 6.5 mg kg^{-1} (18 wt%).

Power (W cm^{-2})	M_{Au} (nmol)	Cp_{Au} (J mol^{-1} k^{-1})	$M_{p\text{-}unit}$ (nmol)	$Cp_{p\text{-}unit}$ (J mol^{-1} k^{-1})	M_{w} (mmol)	Cp_{w} (J mol^{-1} k^{-1})	ΔT (K)	Q_{abs} (J)	Q_{tot} (J)	*PCE* (%)
0.6	91.4	25.42	36.1	205	55.5	75.34	4.9	20.5	72	28.5
1.2	91.4	25.42	36.1	205	55.5	75.34	11.1	46.4	144	32.2
1.5	91.4	25.42	36.1	205	55.5	75.34	14.2	59.4	180	33.3
1.8	91.4	25.42	36.1	205	55.5	75.34	17.7	74.0	216	34.3

M_{Au}: Moles of Au: (18 mg/L × 1 mL × 10^{-6}) / 197 g = 91.4 nmol.

Cp_{Au}: Heat capacity of Au.[1]

$M_{P\text{-unit}}$: Moles of PANI repeat unit: (6.5 mg/L × 1 mL × 10^{-6}) / 180 g = 36.1 nmol

$Cp_{P\text{-unit}}$:Heat capacity of PANI repeat unit.[2]

M_{W}: Moles of water: 1 ml × 1.0 g/mL / 18.01 g = 55.5 mmol.

Cp_{W}: Heat capacity of water.[1]

ΔT: Change in temperature after 10 min irradiation.

Table S1. Parameters for calculation of Q_{abs}, Q_{tot}, PCE of the GNR/PANI sample under different laser power densities in this work. GNR/PANI samples with the same particle concentration (18 mg_{Au} kg^{-1}) were irradiated with an NIR laser at different power densities for 10 min with a laser beam spot of 0.2 cm^2.

GNP type	GNP info.	GNP dose	Laser dose	Ref.
Gold nanoshell	110 nm Si core/10 nm Au shell, PEG	1.5×10^{10} NPs/mL	820 nm, 4 W/cm^2, 6 min	**46**
Gold nanosphere	SiO_2-coated Fe_3O_4 and Au (30nm) nanoparticle	30 mg_{Au}/kg	785 nm, 4.9 W/cm^2, 4 min	**26**
Gold nanorod	aspect ratio of 3.35, PEG	20 mg_{Au}/kg	810 nm, 2 W/cm^2, 5 min	**55**
Gold nanorod	aspect ratio of 3.9, Anti-EGFR conjugated	197 mg_{Au}/kg	800 nm,10 W/cm^2, 4 min	**47**
Gold nanorod	aspect ratio of 2.9, GNR/PANI core-shell nanoparticle	18 mg_{Au}/kg	808 nm, 0.6 W/cm^2, 5 min	**Present work**

Table S2: Comparison of some Au nanoparticle type, laser and nanoparticle doses for cancer photothermal therapy. (Note: A. GNP represents Gold nanoparticle. B. PEG means that the particle is coated with polyethylene glycol. C. PANI means polyaniline)

References for Supporting Information:

1. T. N. Lambert, N. L. Andrews, H. Gerung, T. J. Boyle, J. M. Oliver, B. S. Wilson and S. M. Han, Small, 2007, **3**, 691-699. .

2. A. K. Mishra and P. Tandon, J. Phys. Chem. B, 2009, **113**, 9702-9707.