SUPPORTING INFORMATION

Plasmonic rod-in-shell nanoparticles for photothermal therapy

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Figure S1 shows the dielectric functions of Au and Ag, The dielectric function of Au/Ag alloy is an average of the Au and Ag in the whole wavelength range. The dielectric data of Au is from Christy and Johnson and Ag is from Palik.



Figure S1. The refractive index of (A) Au and (B) Ag.

Figure S2 is the detailed calculation results of the gold nanorod. The black curves are the absorption spectra of the nanorod in transverse polarization and the red curves are corresponding to the longitudinal polarization. As the aspect ratio of the nanorod varies from 3 to 6, the resonance peak in longitudinal polarization is red-shifted. Only when the aspect ratio reaches 6, the resonance peak could be shifted to the second NIR window. The locations of the resonance peak in transverse polarization almost keep the same in the visible region.



Figure S2. Calculated absorption spectra of a gold nanorod (D = 20 nm) with different lengths (L): (i) 60, (ii) 80, (iii) 100, and (iv) 120 nm, when illuminated by the (black) transversely and (red) longitudinally polarized light.



Figure S3. Calculated absorption, scattering and extinction spectra of a Au rod-in-shell particle (D = 20 nm, L = 60 nm, T = 4 nm, G = 5 nm) excited by (A) the transversely and (B) longitudinally polarized light.

Figure S4 shows the calculated absorption spectra of a Au nanorod (D = 38 nm, L = 60 nm) with the same gold mass of a Au rod-in-shell particle (D = 20 nm, L = 60 nm, T = 4 nm, G = 5 nm). By careful comparison, the longitudinal absorption cross section of the RIS in the first NIR window is slightly stronger than the nanorod. But the longitudinal absorption cross-section of the RIS particles in the second NIR window is much greater in intensity than that of the nanorod. Additionally, the transverse absorption response of the RIS particles is also much stronger in the first NIR window.



Figure S4. (A, C) Schematic illustration and (B, D) calculated absorption spectra of (A, B) a Au nanorod (D = 38 nm, L = 60 nm) or (C, D) a Au rod-in-shell particle in the same volume of the nanorod (D = 20 nm, L = 60 nm, T = 4 nm, G = 5 nm) when illuminated by the (black) transversely or (red) longitudinally polarized light. The blue and yellow shaded areas indicate the first and second biological window (window 1 and window 2), respectively.



Figure S5. Calculated absorption spectra of a Au rod-in-shell particle (D = 20 nm, L = 60 nm, T = 4 nm, G = 5 nm) with gap filled with air (black line) and water (red line), and Au rod-in-shell particle (D = 20 nm, L = 60 nm, T = 6 nm, G = 6 nm) with gap filled with water (blue line) excited by (A) the transversely and (B) longitudinally polarized light.