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High spectral field enhancement and tunability in core-double shell metal-dielectric-metal spherical nanoparticles

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Supplementary information

A.1. Determination of the extinction cross sections

Considering a core-double shell nanoparticle as shown in Figure 1, four regions can be defined: $R < R_1$, $R_1 < R < R_2$, $R_2 < R < R_3$ and $R > R_3$, which correspond to the core, the first layer, the second layer and the surrounding media in which the nanoparticle is immersed, respectively. The expression of the incident electric field in terms of spherical vector functions can be written as [25]:

$$E_i = E_0 \sum_{n=1}^{\infty} i^n \frac{2n+1}{n(n+1)} \left(M_{j1n}^{(1)} - i N_{p1n}^{(1)} \right), \qquad \text{(A1.1)}$$

From the continuity conditions of the electric and magnetic fields at each interface, a set of equations can be derived:

$$f_n m_1 \varphi_n(m_2 x) - v_n m_1 \chi_n(m_2 x) - c_n m_2 \varphi_n(m_1 x) = 0 \qquad \text{(A1.2)}$$

$$f_n \varphi'_n(m_2 x) - v_n \chi'_n(m_2 x) - c_n \varphi'_n(m_1 x) = 0$$

$$g_n m_1 \varphi'_n(m_2 x) - w_n m_1 \chi'_n(m_2 x) - d_n m_2 \varphi'_n(m_1 x) = 0$$

$$g_n\varphi_n(m_2x) - w_n\chi_n(m_2x) - d_n\varphi_n(m_1x) = 0$$

$$l_n m_2\varphi_n(m_3y) - p_n m_2\chi_n(m_3y) - f_n m_3\varphi_n(m_2y) + v_n m_3\chi_n(m_2y) = 0$$

$$l_n\varphi'_n(m_3y) - p_n\chi'_n(m_3y) - f_n\varphi'_n(m_2y) + v_n\chi'_n(m_2y) = 0$$

$$o_n m_2\varphi'_n(m_3y) - q_n m_2\chi'_n(m_3y) - g_n m_3\varphi'_n(m_2y) + w_n m_3\chi'_n(m_2y) = 0$$

$$o_n\varphi_n(m_3y) - q_n\chi_n(m_3y) - g_n\varphi_n(m_2y) + w_n\chi_n(m_2y) = 0$$

$$m_3\varphi'_n(z) - a_n m_3\xi'_n(z) - o_n\varphi'_n(m_3z) + q_n\chi'_n(m_3z) = 0$$

$$\varphi_n(z) - a_n\xi_n(z) - o_n\varphi_n(m_3z) + q_n\chi_n(m_3z) = 0$$

$$b_n m_3\xi_n(z) - m_3\varphi_n(z) + l_n\varphi_n(m_3z) - p_n\chi_n(m_3z) = 0$$

$$b_n\xi'_n(z) - \varphi'_n(z) + l_n\varphi'_n(m_3z) - p_n\chi'_n(m_3z) = 0, \qquad \text{(A1.13)}$$

where $m_i = \frac{k_i}{k} = \frac{N_i}{N}$, $k_i = \frac{2\pi N_i}{\lambda}$, $x = kR_1$, $y = kR_2$, $z = kR_3$, $\varphi_n(x) = xj_n(x)$, $\chi_n(x) = xy_n(x)$ and $\xi_n(x) = x\mathrm{h}_n^{(1)}(x) = \varphi_n(x) + i\chi_n(x)$. The solution of the system of equations defined by [A1.2 - A1.13] allows to determine the expressions for a_n and b_n:

$$a_n = \frac{m_3\varphi_n'(z)\left[\varphi_n(m_3z) - Q_n\chi_n(m_3z)\right] - \varphi_n(z)\left[\varphi_n'(m_3z) - Q_n\chi'_n(m_3z)\right]}{m_3\xi_n'(z)\left[\varphi_n(m_3z) - Q_n\chi_n(m_3z)\right] - \xi_n(z)\left[\varphi_n'(m_3z) - Q_n\chi'_n(m_3z)\right]} \qquad \text{(A1.14)}$$

$$b_n = \frac{m_3\varphi_n(z)\left[\varphi_n'(m_3z) - P_n\chi'_n(m_3z)\right] - \varphi_n'(z)\left[\varphi_n(m_3z) - P_n\chi_n(m_3z)\right]}{m_3\xi_n(z)\left[\varphi_n'(m_3z) - P_n\chi'_n(m_3z)\right] - \xi_n'(z)\left[\varphi_n(m_3z) - P_n\chi_n(m_3z)\right]}$$

$$P_n = \frac{p_n}{l_n} = \frac{m_3\varphi_n'(m_3y)\left[\varphi_n(m_2y) - V_n\chi_n(m_2y)\right] - m_2\varphi_n(m_3y)\left[\varphi_n'(m_2 \ldots\right.}{m_3\chi_n'(m_3y)\left[\varphi_n(m_2y) - V_n\chi_n(m_2y)\right] - m_2\chi_n(m_3y)\left[\varphi_n'(m_2 \ldots\right.}$$

$$Q_n = \frac{q_n}{o_n} = \frac{m_3\varphi_n(m_3y)\left[\varphi_n^{'}(m_2y) - W_n\chi'_n(m_2y)\right] - m_2\varphi_n^{'}(m_3y)\left[\varphi_n(m\right.}{m_3\chi_n(m_3y)\left[\varphi_n^{'}(m_2y) - W_n\chi'_n(m_2y)\right] - m_2\chi_n^{'}(m_3y)\left[\varphi_n(m\right.}$$

$$V_n = \frac{v_n}{f_n} = \frac{m_2\chi_n(m_1x)\varphi_n^{'}(m_2x) - m_1\varphi_n(m_2x)\varphi_n^{'}(m_1x)}{m_2\chi_n(m_1x)\varphi_n^{'}(m_2x) - m_1\varphi_n(m_2x)\varphi_n^{'}(m_1x)}$$

$$W_n = \frac{w_n}{g_n} = \frac{m_2\varphi_n(m_2x)\varphi_n^{'}(m_1x) - m_1\varphi_n(m_1x)\varphi_n^{'}(m_2x)}{m_2\chi_n(m_2x)\varphi_n^{'}(m_1x) - m_1\varphi_n(m_1x)\chi_n^{'}(m_2x)} \quad \text{(A1.19)}$$

When the particle size is small compared to the wavelength $m_1x, m_2y, m_3z, x, y, z \ll 1$, extinction, scattering and absorption cross sections are described by equations [7] and [8], where

$$\alpha = 4\pi c^3 \frac{\alpha_1 + \alpha_2}{\alpha_3 + \alpha_4}$$

$$\alpha_1 = (\varepsilon_1 + 2\varepsilon_2)(\varepsilon_2 - \varepsilon_3)(2\varepsilon_3 + \varepsilon_m)f + (2\varepsilon_2 + \varepsilon_1)(2\varepsilon_3 + \varepsilon_2)(\varepsilon_3 - \varepsilon_m)$$

$$\alpha_2 = 2(\varepsilon_2 - \varepsilon_1)(\varepsilon_3 - \varepsilon_2)(\varepsilon_3 - \varepsilon_m)g + (\varepsilon_1 - \varepsilon_2)(\varepsilon_3 + 2\varepsilon_2)(2\varepsilon_3 + \varepsilon_m)h$$

$$\alpha_3 = (\varepsilon_1 + 2\varepsilon_2)(\varepsilon_2 - \varepsilon_3)(2\varepsilon_3 - 2\varepsilon_m)f + (2\varepsilon_2 + \varepsilon_1)(2\varepsilon_3 + \varepsilon_2)(\varepsilon_3 + 2\varepsilon_m)$$

$$\alpha_4 = 2(\varepsilon_2 - \varepsilon_1)(\varepsilon_3 - \varepsilon_2)(\varepsilon_3 + 2\varepsilon_m)g + (\varepsilon_1 - \varepsilon_2)(\varepsilon_3 + 2\varepsilon_2)(2\varepsilon_3 - 2\varepsilon_m)h \quad \text{(A1.23)}$$

where ε_1, ε_2 and ε_3 are the dielectric functions of each region of the nanoparticle, and ε_m is the dielectric function of the surrounding medium. $f = (R_2/R_3)^3$, $g = (R_1/R_2)^3$ and $h = (R_1/R_3)^3$.

A2. M and N spherical vector functions

Functions M_{j1n}, M_{p1n}, N_{j1n} y N_{p1n}, used in electric and magnetic fields are described in the form:

$$M_{j1n} = -\sin\phi \pi_n(\theta) z_n(\rho) a_\theta - \sin\phi \tau_n(\theta) z_n(\rho) a_\phi$$

$$M_{p1n} = \cos\phi \pi_n(\theta) z_n(\rho) a_\theta - \sin\phi \tau_n(\theta) z_n(\rho) a_\phi$$

$$N_{j1n} = \cos\phi n(n+1) \sin\theta \pi_n(\theta) \frac{z_n(\rho)}{\rho} a_r + \cos\phi \tau_n(\theta) \frac{[\rho z_n(\rho)]'}{\rho} a_\theta - \sin\phi \pi_n(\theta) \frac{[\rho z_n(\rho)]'}{\rho} a_\phi$$

$$N_{p1n} = \sin\phi n(n+1) \sin\theta \pi_n(\theta) \frac{z_n(\rho)}{\rho} a_r + \sin\phi \tau_n(\theta) \frac{[\rho z_n(\rho)]'}{\rho} a_\theta + \cos\phi \pi_n(\theta) \frac{[\rho z_n(\rho)]'}{\rho} a_\phi \quad \text{(A.2.1)}$$

where $\pi_n(\theta) = P_n^1(\cos\theta)/\sin\theta$ and $\tau_n(\theta) = dP_n^1(\cos\theta)/d\theta$. $P_n^1(\cos\theta)$ are the associated Legendre polynomials.