

Supplemental Information

## DDA simulations of noble metal and their alloy nanocubes for tunable optical properties in biological imaging and sensing

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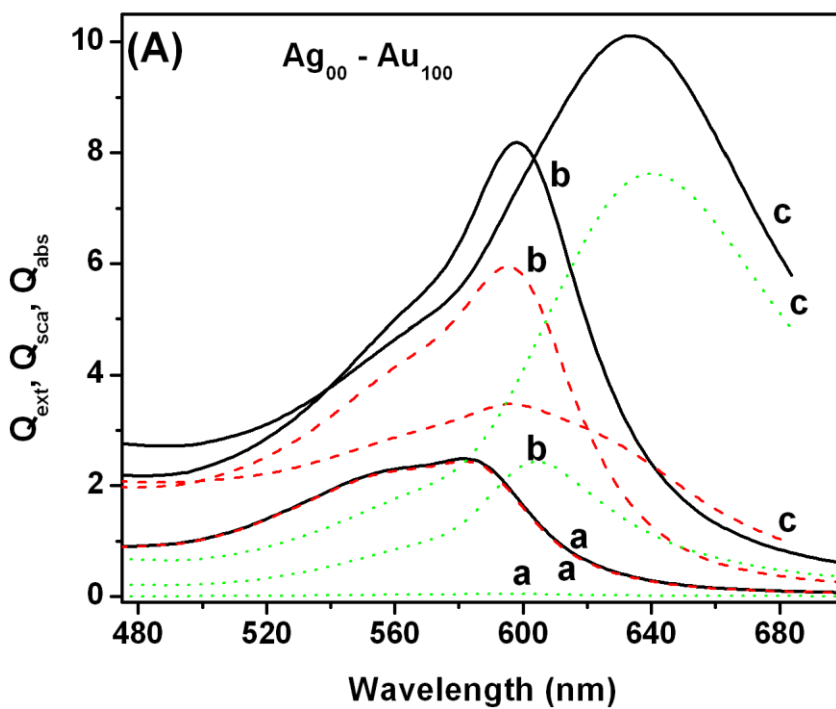


Figure S1A

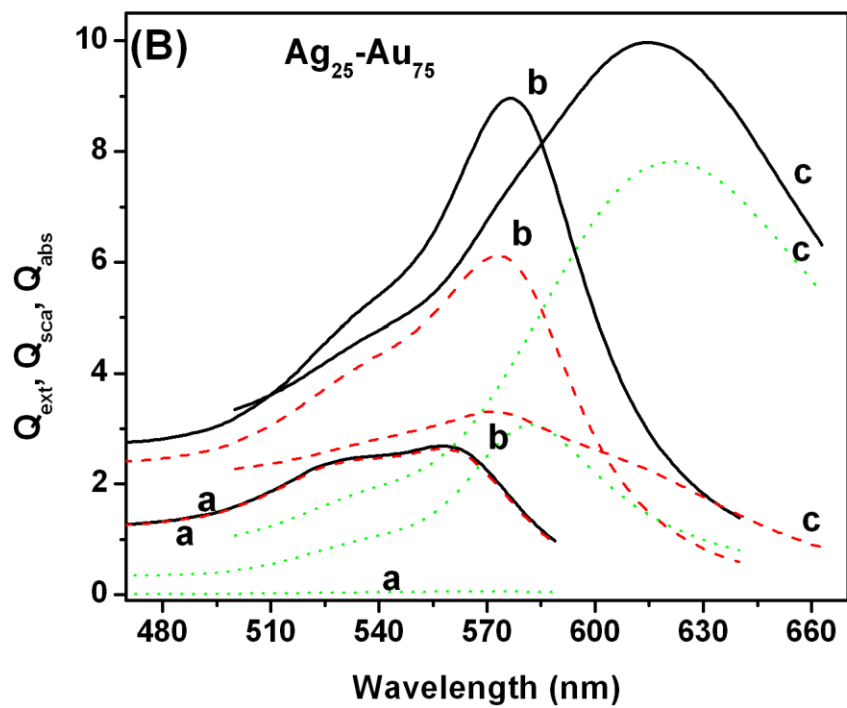


Figure S1B

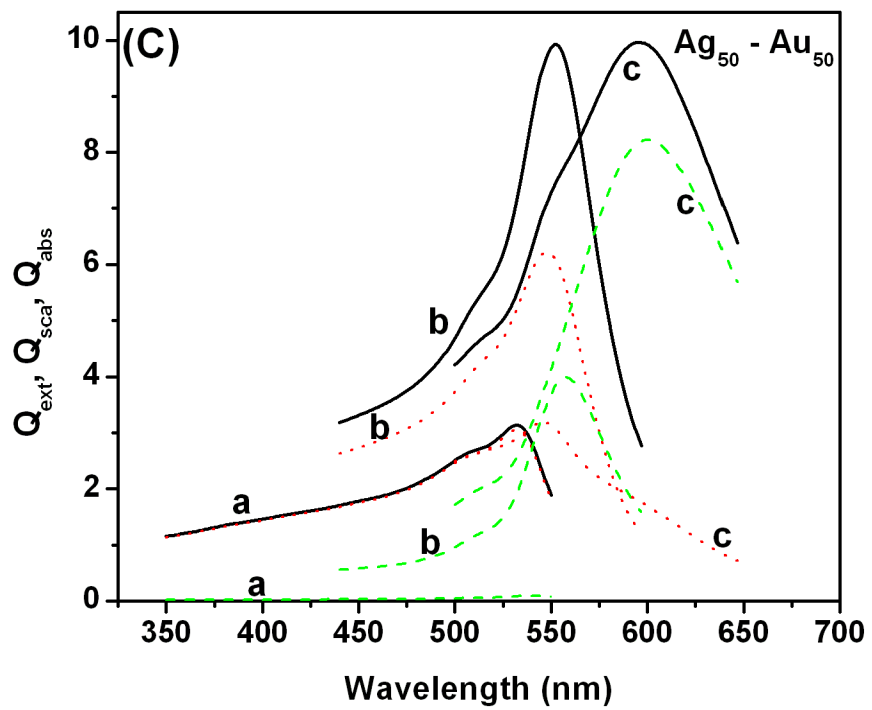


Figure S1C

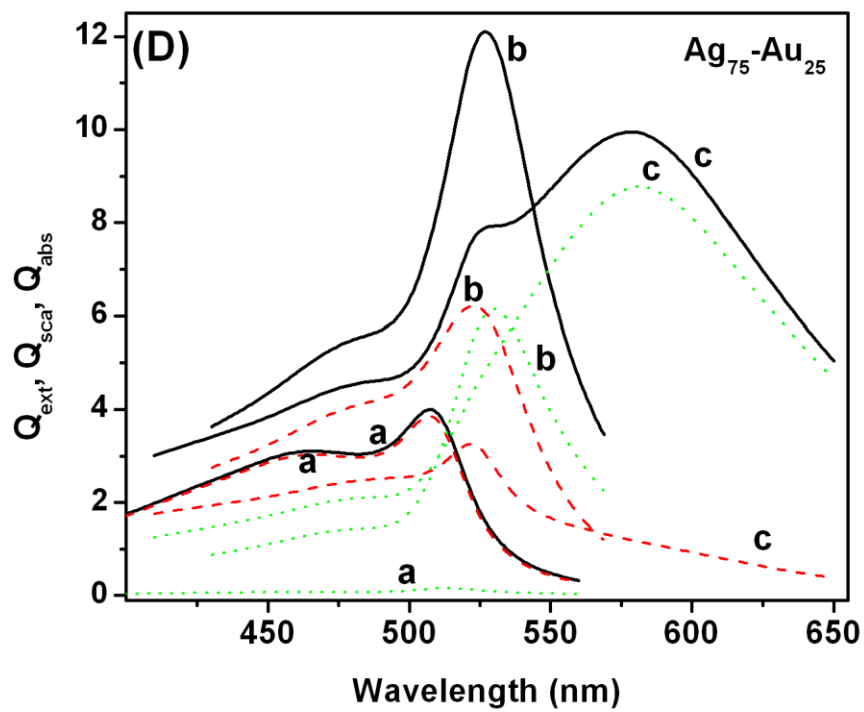


Figure S1D

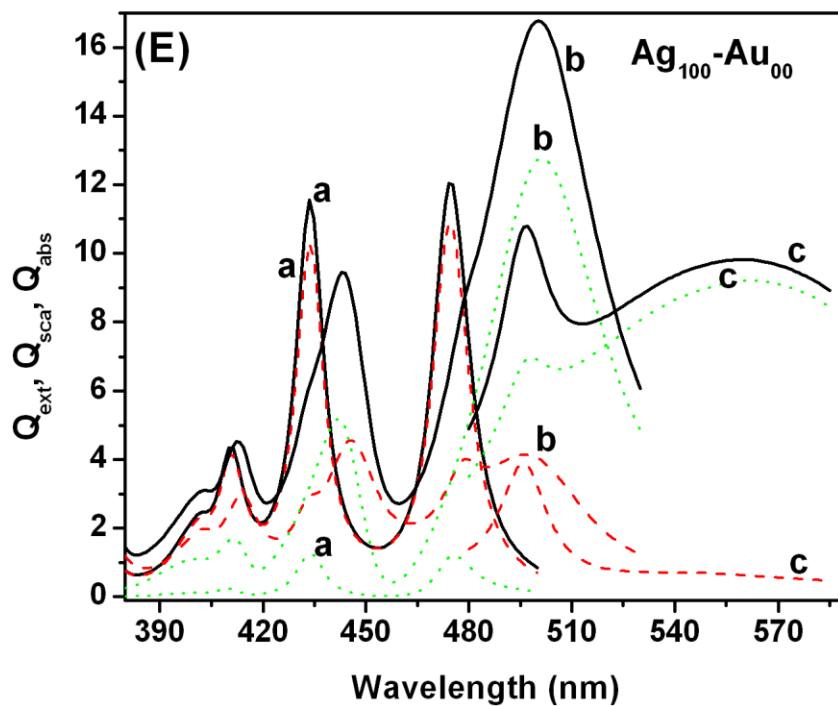
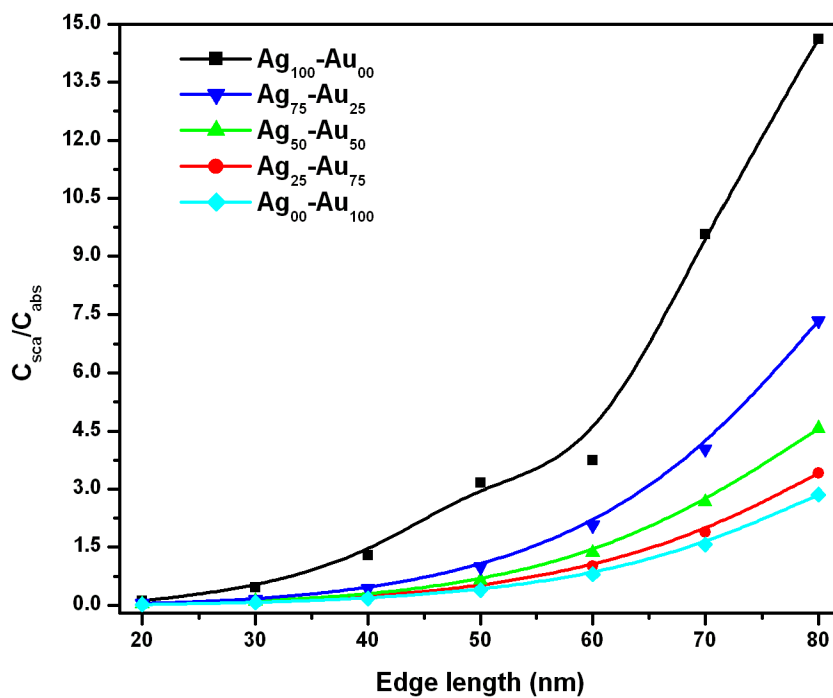
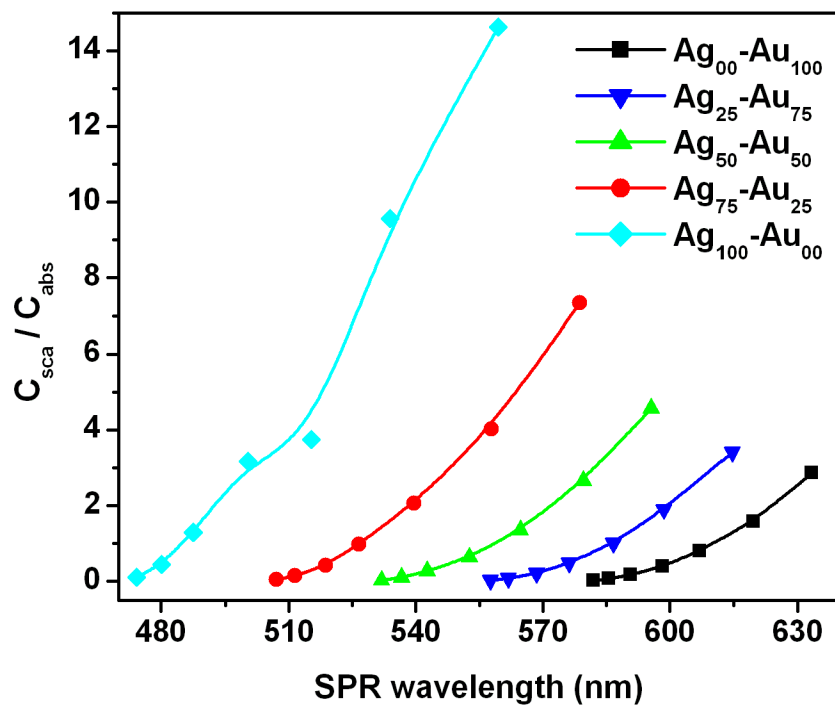


Figure S1E

**Figure S1:** Calculated efficiency spectra of extinction  $Q_{\text{ext}}$  (solid black lines), scattering  $Q_{\text{sca}}$  (dotted green lines), and  $Q_{\text{abs}}$  (dashed red lines) for edge length of (a) 20 nm; (b) 50 nm; (c) 80 nm of (A)  $\text{Ag}_{00}\text{-Au}_{100}$  (B)  $\text{Ag}_{25}\text{-Au}_{75}$  (C)  $\text{Ag}_{50}\text{-Au}_{50}$  (D)  $\text{Ag}_{75}\text{-Au}_{25}$  (E)  $\text{Ag}_{100}\text{-Au}_{00}$  alloys nanocubes.



**Figure S2:** Variation in  $C_{sca}/C_{abs}$  of nanocubes with nanocube edge length.



**Figure S3:** Variation in  $C_{sca}/C_{abs}$  of nanocubes with SPR wavelength.

**Table S1:** Calculated SPR wavelength (nm), ratio of scattering to absorption efficiency, refractive index sensitivity (nm/RIU) and FOM for Au, Au<sub>75</sub>-Ag<sub>25</sub>, Au<sub>50</sub>-Ag<sub>50</sub>, Au<sub>25</sub>-Ag<sub>75</sub>, Ag nanocubes of different width

Width (nm)	$\lambda_{\text{SPR}}$ (nm)	$Q_{\text{sca}}/Q_{\text{abs}}$	RIS (nm/RIU)	FOM
	Au, Au <sub>75</sub> -Ag <sub>25</sub> , Au <sub>50</sub> -Ag <sub>50</sub> , Au <sub>25</sub> -Ag <sub>75</sub> , Ag	Au, Au <sub>75</sub> -Ag <sub>25</sub> , Au <sub>50</sub> -Ag <sub>50</sub> , Au <sub>25</sub> -Ag <sub>75</sub> , Ag	Au, Au <sub>75</sub> -Ag <sub>25</sub> , Au <sub>50</sub> -Ag <sub>50</sub> , Au <sub>25</sub> -Ag <sub>75</sub> , Ag	Au, Au <sub>75</sub> -Ag <sub>25</sub> , Au <sub>50</sub> -Ag <sub>50</sub> , Au <sub>25</sub> -Ag <sub>75</sub> , Ag
20	581.9, 557.6, 531.91, 507.12, 474.26	0.02, 0.02, 0.03, 0.04, 0.11	170.82, 314.35, 362.6, 161.75, 209.65	1.84, 3.16, 2.75, 1.43, 1.78
30	585.7, 561.8, 536.64, 511.53, 480.11	0.07, 0.08, 0.10, 0.14, 0.45	176.0, 300.37, 360.2, 167.91, 219.52	2.0, 3.43, 3.69, 1.83, 3.86
40	590.7, 568.6, 542.73, 518.68, 487.52	0.17, 0.21, 0.27, 0.42, 1.3	188.11, 282.38, 275.12, 178.72, 234.68	2.27, 3.51, 3.55, 2.57, 3.58
50	598.2, 576.2, 552.7, 526.57, 500.31	0.39, 0.48, 0.64, 0.98, 3.16	195.24, 274.95, 221.1, 188.95, 256.22	2.43, 3.48, 2.89, 3.41, 3.08
60	607.0, 586.7, 564.68, 539.58, 513.38	0.8, 1.0, 1.35, 2.06, 3.75	206.99, 277.37, 223.79, 204.6, 276.44	2.46, 3.29, 2.92, 4.21, 2.8
70	619.6, 598.6, 579.64, 557.81, 533.87	1.57, 1.89, 2.66, 4.08, 9.57	225.92, 294.9, 239.37, 232.06, 301.48	2.34, 2.94, 2.64, 2.43, 2.65
80	633.4, 614.6, 595.64, 578.73, 559.49	2.85, 3.41, 4.57, 7.33, 14.62	246.77, 302.7, 264.99, 260.66, 338.48	2.18, 2.6, 2.18, 1.78, 3.28