Electronic Supplementary Information

Large-volume hot spots in gold spiky nanoparticle dimers for high-performance surface-enhanced spectroscopies

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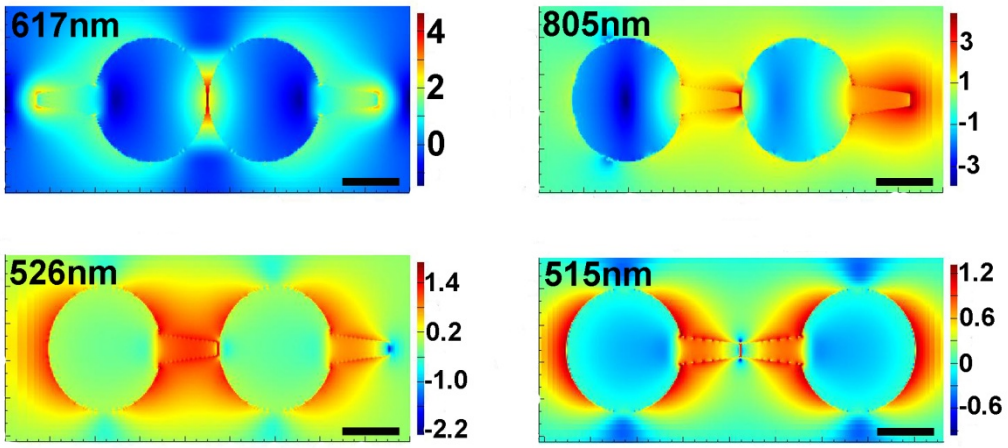

Fig. S1. Electric field distribution ($\log_{10}|E|^2/|E_0|^2$) of the sphere to sphere, tip to sphere and tip to tip spiky nanoparticle dimers at their corresponding resonant peaks. The scale bar in each figure is 50 nm.

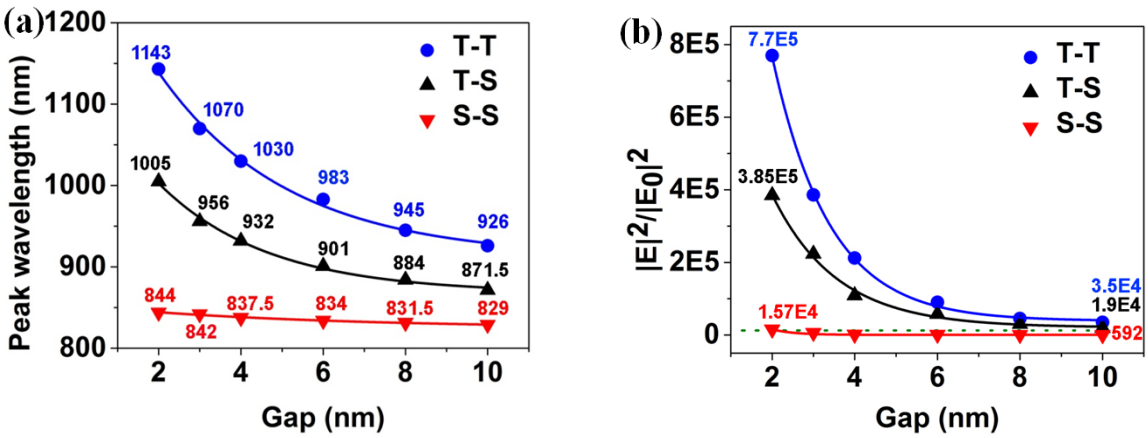

Fig. S2. (a) Peak wavelength as a function of gap sizes for sphere-to-sphere (S-S), tip-to-sphere (T-S) and tip-to-tip (T-T) spiky nanoparticle dimers (SNPDs). (b) Electric field enhancement ($|E|^2/|E_0|^2$) at the gap center of three SNPDs under corresponding resonant conditions as a function of gap sizes. The solid lines in (a) and (b) show the exponential fitting results. The dashed green line in (b) shows the maximum electric field enhancement (1.25×10^4) at the spike side of single SNP when the incidence polarization is along its long axis.

Table S1. Exponential fitting ($y(x)=A_0*exp(-x/D_0)+C$) results for the peak wavelength shift as a function of gap separations for various dimer structures.

structure	A_0 (nm)	D_0 (nm)	C (nm)	*R-square*
T-T SND	430.726	3.133	911.551	0.99301
T-S SND	285.785	2.665	867.856	0.99355
S-S SND	28.474	5.476	824.559	0.98287

Table S2. Exponential fitting results ($y(x)=A_0*exp(-x/D_0)+C$) for the electric field enhancement ($|E|^2/|E_0|^2$) at the center of dimer gaps as a function of gap separations for various dimer structures.

structure	A_0 (nm)	D_0 (nm)	C (nm)	*R-square*
T-T SND	$3.11x10^6$	1.380	$3.88x10^4$	0.99913
T-S SND	$1.31x10^6$	1.564	$2.09x10^4$	0.99375
S-S SND	$6.47x10^5$	0.532	$5.92x10^2$	0.8732

Table S3. Calculated maximum electric field enhancement ($|E|^2/|E_0|^2$) for gold crossed T-T SNPDs with different core diameters ranging from 50 nm to 400 nm at their individual resonant conditions.

Crossed T-T SNPD (x=25 nm)	resonant wavelength (nm)	Maximum ($|E|^2/|E_0|^2$)
d=50	980	$2.04x10^5$
d=100	1173	$5.68x10^5$
d=200	1343	$9.94x10^5$
d=300	1468	$8.64x10^5$
d=400	1675	$5.14x10^5$

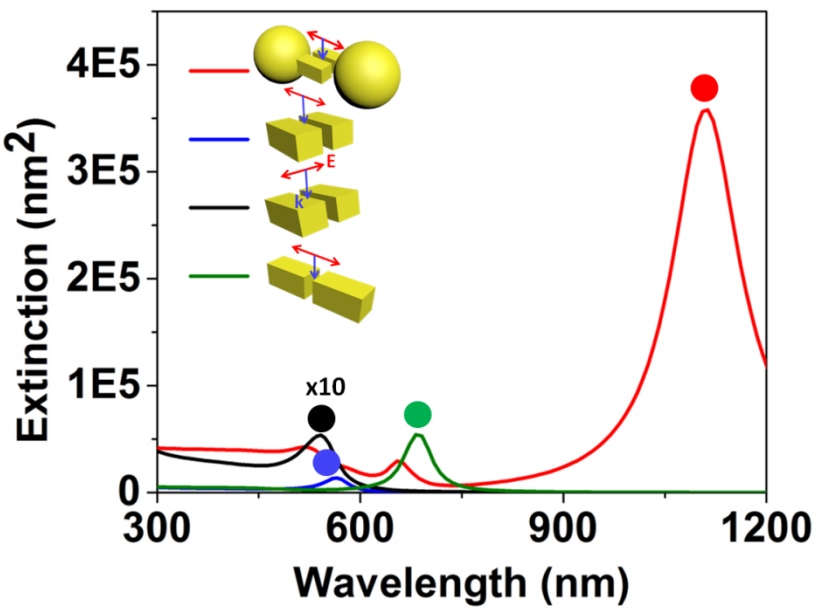

Fig. S3. Extinction spectra for cuboid dimers with different configurations. The black line is multiplied by 10 to show clearly. The solid circles represent the resonant peak used to calculate the electric field distribution shown in Fig. 5.

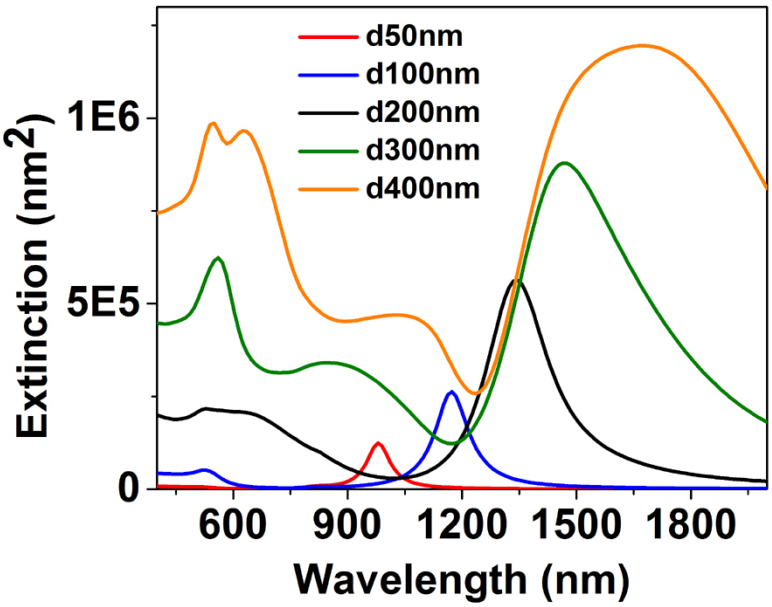

Fig. S4. Extinction spectra of crossed tip-to-tip spiky nanoparticle dimers with different spherical core sizes. The tip-to-tip overlap for each dimer is 25 nm.