Electronic supplementary information (ESI)

Determination of Ion Pairing on Capping Structures of Gold Nanoparticles by Phase Extraction

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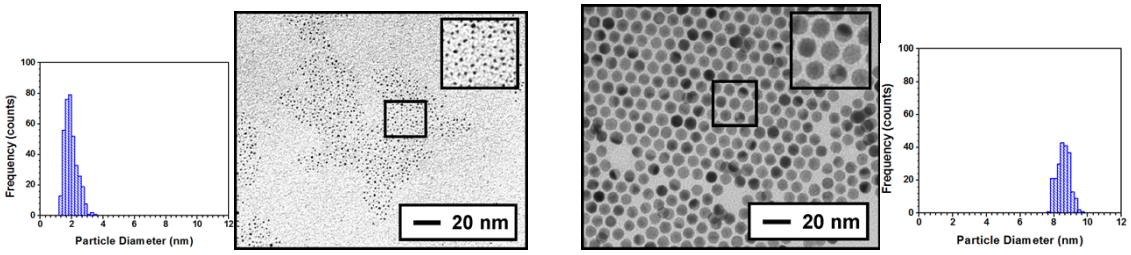
Additional Experimental Details:

Table S1. Data from the determination of MUA ligand ion pairing in mixed monolayer $Au_{2nm}(DT)_x(MUA^-)_y$ by TOA^+.

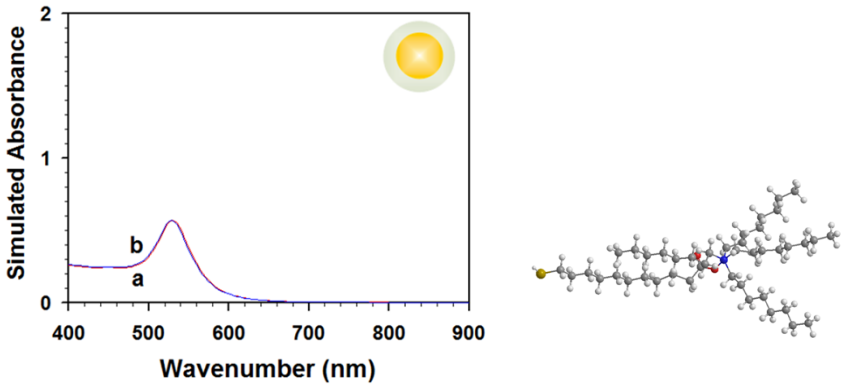
Titration (Trial #)	[a] $Au_{2.0nm}(DT)_x(MUA^-)_y$ (μ moles)	[b] TOA^+Br^- (μ moles)	[c] % MUA in ligand shell
1	0.085	3.75	51.2
2	0.170	7.00	47.6
3	0.170	6.75	45.9

a) Calculated from the Au mass & the TEM-determined size; b) Determined the phase extraction; c) volumetric titration errors: ±1%.



(a) (b)

Figure S1 TEM and size distributions for (a) $Au_{2.0nm}(DT)$ and (b) $Au_{8.5nm}(DT)$ nanoparticles.



(A) (B)

Figure S2. (A) Simulation of the SP band for $Au_{2.0nm}(DT)_x(MUA^-)_{100-x}$ in the aqueous phase (a) and $Au_{2nm}(DT)_x(MUA^-)_{100-x}(TOA^+)_{n\ y}$ in the toluene phase (b). (The refractive indexes for aqueous phase (1.330), capping agent DT/MUA (1.475), TOA-MUA (1.446), and toluene phase (1.496)). (B) Model for estimate of the molecular size and shape of TOA^+ for $Au_{nm}(DT)_x(MUA^-)_{100-x}(TOA^+)_n$: For 1 DT area: $\pi(1.546+1Å)^2$= 0.20 nm^2; # of DTs on $Au_{2.0nm}(DT)$: $4\pi nm^2/\ \pi(2.55x10^{-1}nm)^2$= 62; 1 TOA-MUA area: $\pi(8.30+1Å)^2$= 2.72 nm^2; 1 Au2nm-DT core-shell sphere: $4\pi(1+1.55\ nm)^2$= 81.53 nm^2; # of TOA-MUA on Au2nm-DT core-shell sphere: 81.53 nm^2/2.72 nm^2= 30; The % of TOA-MUA vs. original DTs $Au_{2.0nm}(DT)$: 30 /62 = 48%.