nanomaterials

Supplementary Materials

Simple Determination of Gold Nanocrystal Dimensions by Analytical Ultracentrifugation via Surface Ligand-Solvent Density Matching

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1. Derivation of the Svedberg Equation for NC@SL@SS

The interplay of three forces governs the sedimentation behaviour of a NC@SL@SS: i) the applied centrifugal force ($F_{s,NC@SL@SS,}$), ii) the buoyant force ($F_{b,NC@SL@SS}$), and iii) the frictional force ($F_{f,NC@SL@SS}$) (eqs. 7, 8 and 9 in the main text). Note that all eqs. follow the indexation given in the main text.

$$F_{f,NC@SL@SS} = -f_{NC@SL@SS} \cdot u \tag{7}$$

$$F_{s,NC@SL@SS} = \omega^2 \cdot r \cdot (m_{NC} + m_{SL} + m_{SS}) \tag{8}$$

$$F_{b,NC@SL@SS} = -\omega^2 \cdot r \cdot \rho \cdot \left(m_{NC} \cdot \frac{1}{\rho_{NC}} + m_L \cdot \frac{1}{\rho_{SL}} + m_S \cdot \frac{1}{\rho_{SS}}\right) \tag{9}$$

During the sedimentation experiment, a balance between the three forces is reached (eq. 10 in the main text):

$$F_{s,NC@SL@SS} + F_{b,NC@SL@SS} = F_{f,NC@SL@SS} \tag{10}$$

and by insertion of (4), (7), (8), and (9) in (10):

$$\omega^2 \cdot r \cdot (m_{NC} + m_{SL} + m_{SS}) - \omega^2 \cdot r \cdot \rho \cdot \left(m_{NC} \cdot \frac{1}{\rho_{NC}} + m_{SL} \cdot \frac{1}{\rho_{SL}} + m_{SS} \cdot \frac{1}{\rho_{SS}}\right) = \frac{kT}{D_{NC@SL@SS}} \cdot u \tag{S1}$$

$$\omega^2 \cdot r \cdot \left[(m_{NC} + m_{SL} + m_{SS}) - \rho\left(m_{NC} \cdot \frac{1}{\rho_{NC}} + m_{SL} \cdot \frac{1}{\rho_{SL}} + m_{SS} \cdot \frac{1}{\rho_{SS}}\right)\right] = \frac{kT}{D_{NC@SL@SS}} \cdot u \tag{S2}$$

$$\frac{D_{NC@SL@SS}\left[(m_{NC} + m_{SL} + m_{SS}) - \rho\left(m_{NC} \cdot \frac{1}{\rho_{NC}} + m_{SL} \cdot \frac{1}{\rho_{L}} + m_{SS} \cdot \frac{1}{\rho_{S}}\right)\right]}{kT} =\cdot \frac{u}{\omega^2 \cdot r} \cdot \tag{S3}$$

Where u/ω^2r is the sedimentation coefficient of the NC@SL@SS, $s_{NC@SL@SS}$

$$s_{NC@SL@SS} = \frac{D_{NC@SL@SS}\left[(m_{NC} + m_{SL} + m_{S}) - \rho\left(m_{NC} \cdot \frac{1}{\rho_{NC}} + m_{L} \cdot \frac{1}{\rho_{L}} + m_{S} \cdot \frac{1}{\rho_{S}}\right)\right]}{kT} \tag{S4}$$

$$s_{NC@SL@SS} = \frac{D_{NC@SL@SS}\left[m_{NC} \cdot \left(1 - \frac{\rho}{\rho_{NC}}\right) + m_{SL} \cdot \left(1 - \frac{\rho}{\rho_{SL}}\right) + m_{SS} \cdot \left(1 - \frac{\rho}{\rho_{SS}}\right)\right]}{kT} \tag{S5}$$

Where k=R/N_A (N_A = Avogadros constant), and thus, we arrive at the final form of the Svedberg equation for NC@SL@SS (11)

$$s_{NC@SL@SS} = \frac{D_{NC@SL@SS} \cdot N_A\left[m_{NC} \cdot \left(1 - \frac{\rho}{\rho_{NC}}\right) + m_{SL} \cdot \left(1 - \frac{\rho}{\rho_{SL}}\right) + m_{SS} \cdot \left(1 - \frac{\rho}{\rho_{SS}}\right)\right]}{R \cdot T} \tag{11}$$

And since M = m N_A

$$s_{NC@SL@SS} = \frac{D_{NC@SL@SS} \cdot \left[M_{NC} \cdot \left(1 - \frac{\rho}{\rho_{NC}}\right) + M_{SL} \cdot \left(1 - \frac{\rho}{\rho_{SL}}\right) + M_{SS} \cdot \left(1 - \frac{\rho}{\rho_{SS}}\right)\right]}{R \cdot T} \tag{S6}$$

Or

$$\left[M_{NC} \cdot (1 - \bar{v}_{NC}\,\rho) + M_{L} \cdot (1 - \bar{v}_{SL}\,\rho) + M_{S} \cdot (1 - \bar{v}_{SS}\,\rho)\right] = \frac{s_{NC@SL@SS} \cdot R\,T}{D_{NC@SL@SS}} \tag{S7}$$

2. 3D Plot of Sedimentation Coefficient and $(f/f_c)_{AuNC@CTAB@W}$ (lower) Distributions Obtained at Different Wavelengths.

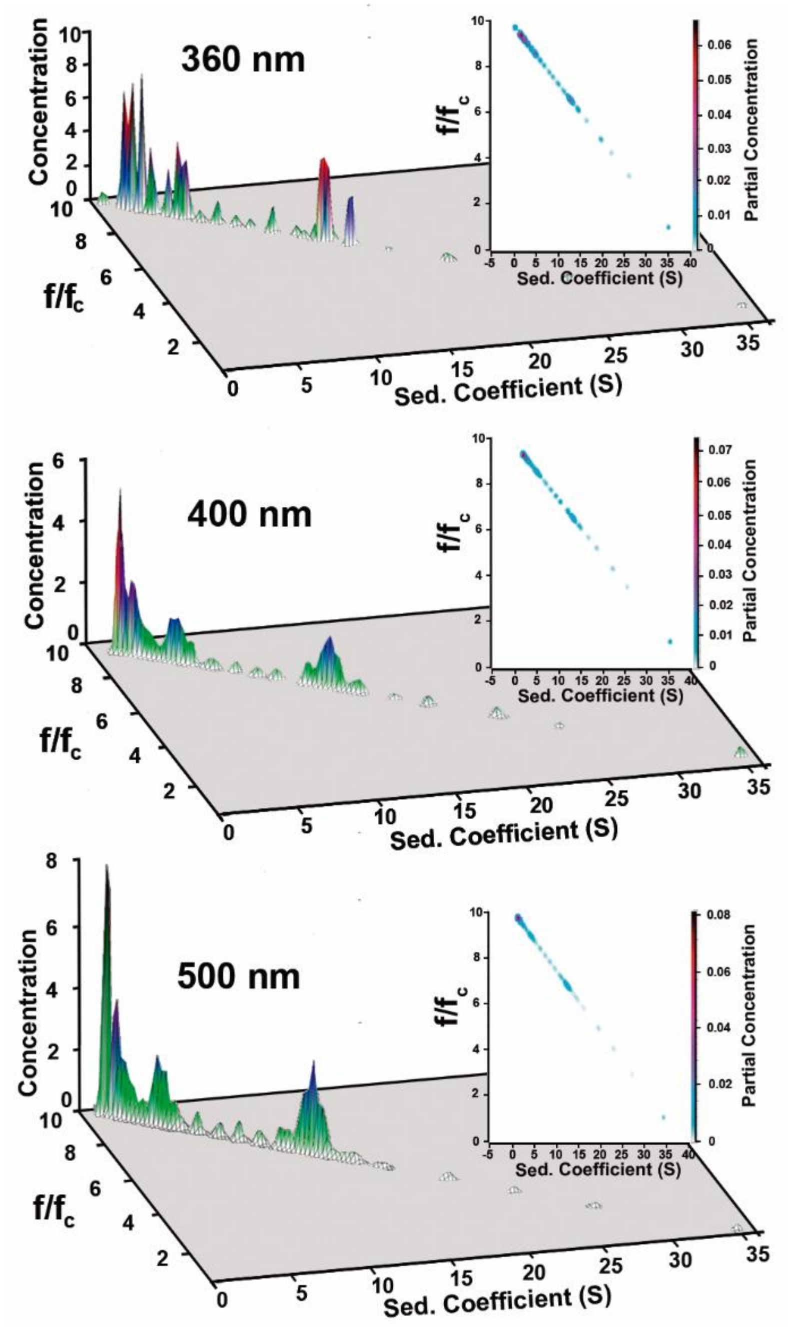

Figure S1. 3D and 2D (inset) plots of sedimentation coefficient and $(f/f_c)_{AuNC@CTAB@W}$ (lower) distributions obtained from sedimentation velocity AUC measurements at 360, 400 and 500 nm (using the density of Au to perform the analysis).