

Supporting Information

Chemical Interface Damping as an Indicator for Hexadecyltrimethylammonium Bromide Replacement by Short-Chain Thiols on Gold Nanorods

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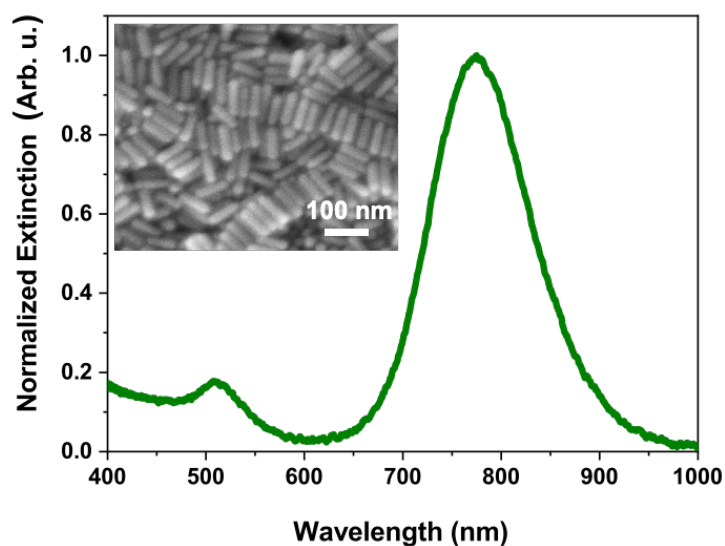


Figure S1. Ensemble extinction spectrum of the as-synthesized gold nanorods. The inset shows a characteristic SEM image of the particles with the dimensions of 76 x 24 nm.

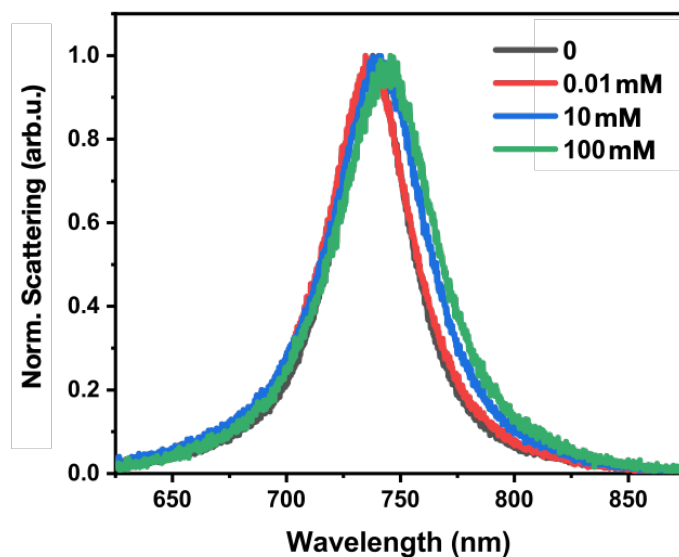


Figure S2. Normalized single particle scattering spectrum of a selected individual gold nanorod obtained at increasing cysteamine concentrations (no CTAB in the bulk).

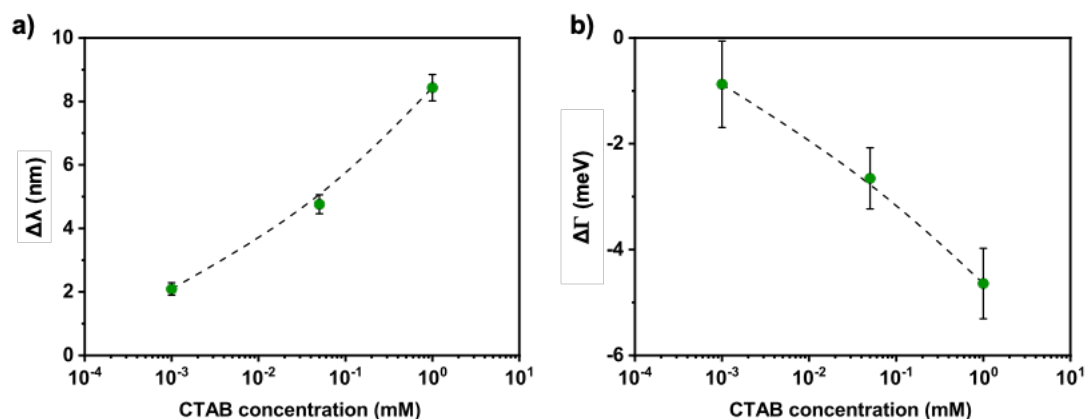


Figure S3. Redshift of the longitudinal plasmon peak (a) and damping change (b) of the nanorods after conditioning them in CTAB solutions ($\Delta\lambda=0$ for the reference samples where the bulk CTAB concentration is set to zero).

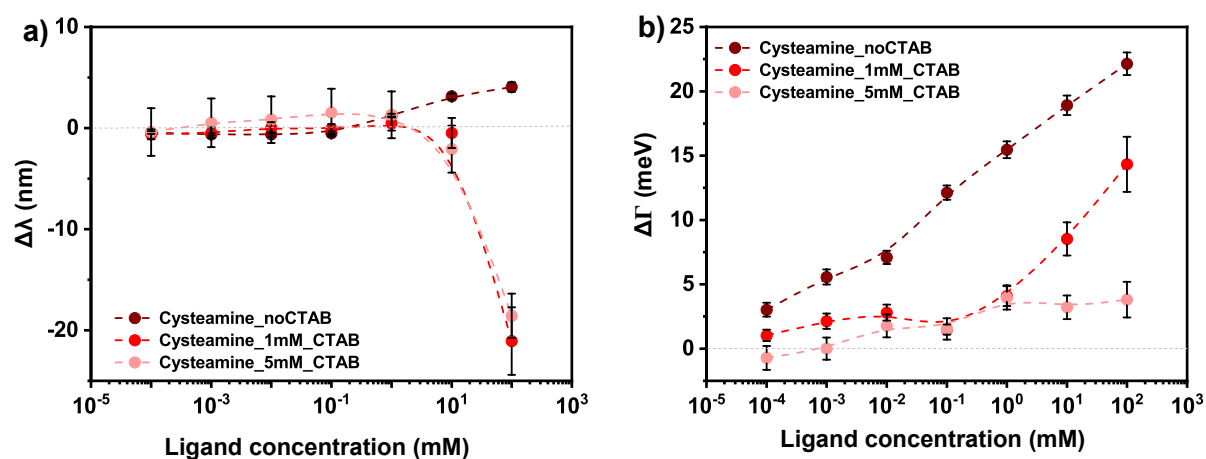


Figure S4. Resonance peak wavelength (a) and damping change (b) when cysteamine is added to the cleaned samples and to ones that have been first conditioned in aqueous CTAB solution.

Simulated single particle scattering spectra

The optical simulations of the nanorods were implemented in Matlab®, using the MNPBEM toolbox.¹ The nanorods were modelled as two hemisphere capped cylinders and the dielectric function of gold was taken from Olmon et al.² The particles were illuminated by a planewave with a wavelength between 620 and 850 nm polarized along the direction to the long-axis of the nanorods (see inset scheme). For simplicity, the presence of the substrate is neglected and the refractive index of the embedding medium is set to 1.33 (water).

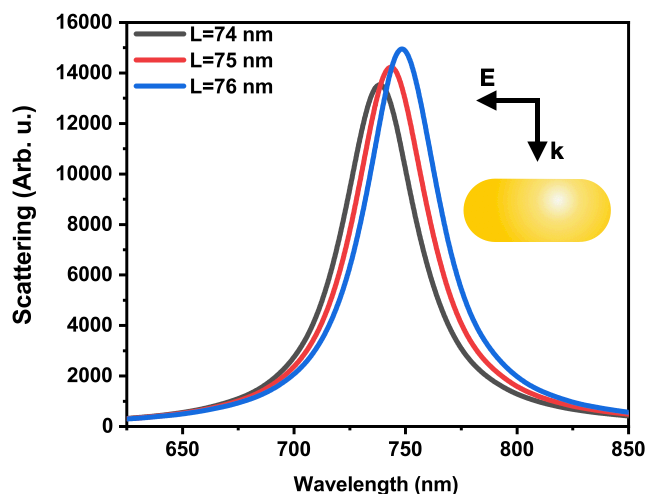


Figure S5. Calculated scattering spectra of a nanorod with 24 nm thickness and various lengths from 76 to 74 nm. The length change corresponds to a change of ca. 0.08 in the aspect ratio.

References:

- (1) Hohenester, U.; Trügler, A. MNPBEM – A Matlab Toolbox for the Simulation of Plasmonic Nanoparticles. *Comput. Phys. Commun.* **2012**, *183* (2), 370–381. <https://doi.org/10.1016/j.cpc.2011.09.009>.
- (2) Olmon, R. L.; Slovick, B.; Johnson, T. W.; Shelton, D.; Oh, S.-H.; Boreman, G. D.; Raschke, M. B. Optical Dielectric Function of Gold. *Phys. Rev. B* **2012**, *86* (23). <https://doi.org/10.1103/PhysRevB.86.235147>.