Supplemental Information

Quasi-fractal gold nanoparticles in Raman spectroscopy: effect of nanoparticle morphology and concentration

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1. Calculations of the isoperimetric ratios using ImageJ software (Figure S1)

ImageJ (v1.52e) processing was performed on raw TEM image files (.dm3), as shown in Figure S1a. The images were first made binary (Process > Binary > Make Binary) (Fig. S1b). This black and white image was then eroded (Process > Binary > Erode) at most three times to (Fig. S1c) accentuate the spaces between nanoparticles and eliminate dark area artifacts that appear as solid black after the binary conversion process. The in-between spaces were then filled (Process > Binary > Fill Holes) (Fig. S1d), followed by using the Flood Fill Tool to eliminate overlapping nanoparticle structures and other artifacts (Fig. S1e). Where possible, when the Erode tool is still does not remove all artifacts, the straight line tool may be employed to pronounce nanoparticle boundaries. The remaining structures are then analyzed (Analyze > Analyze Particles), with outlines shown (Fig. S1f) to ensure that data can be compared to real structures and remaining pixel-sized artifacts may be excluded. The resulting particle perimeters and areas were then utilized to calculate the isoperimetric ratio for all nanoparticles, with calculated isoperimetric ratios then averaged for each synthesis temperature.

2. X-ray diffraction patterns of Au nanoparticles (Figure S2)

The X-ray diffraction patters of synthesized gold nanospheres and of samples synthesized at 25°C (star-like nanparticles) and at 65°C (quasi-fractal nanoparticles) exhibited the diffraction peaks from the (1 1 1), (2 0 0), (2 2 0) and (3 1 1) crystal planes. While the position of the peaks is identical in all three sample, the ratios among the various are slightly, however not different enough to be considered analytically significant.



Figure S1: ImageJ processing of a TEM image. (a) Raw TEM image, (b) Image made binary, (c) Eroded binary image, (d) Hole filling applied to binary image, (e) Manual filling of select regions, and (f) Binary skeleton showing analyzed particles.



Figure S2: The X-ray diffraction pattern of as-synthesized gold nanoparticles. Black spectrum: Au nanospheres. Red Spectrum: Au star-like nanoparticles synthesized at 25°C. Blue spectrum: Au quasi-fractal nanoparticles synthesized at 65°C. The spectra have been spaced in the y-axis (intensity counts) for viewing convenience (with the preservation of the peak heights).