

## Electronic Supplementary Information: Formation of dynamic aggregates in water by cucurbit[5]uril capped with gold nanoparticles

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### 1 Experimental procedure

**Instrumentation** UV-vis studies were performed on a Varian Cary 4000 UV-Vis spectrophotometer. Transmission electron microscopy (TEM) characterization was carried out by a JEOL 2000FX TEM under an accelerating voltage of 200 kV. Samples were prepared by applying one drop of the as-synthesized gold nanoparticles in 50 % (v / v) aqueous ethanol onto a Holey<sup>®</sup> carbon coated copper TEM grid (400 mesh). Dynamic light scattering (DLS) data was obtained on a Malvern Zetasizer Nano S at 20 °C. Fourier-transform infrared spectroscopy (FT-IR) was done on a Perkin Elmer spectrum 100 series with a universal ATR attachment installed. Measurements were done on solid samples with a resolution of 1 cm<sup>-1</sup> for 30 scans per sample.

**Materials** Gold(III) chloride trihydrate and sodium borohydride were purchased from Sigma Aldrich and Alfa Aesar respectively and were used as received.

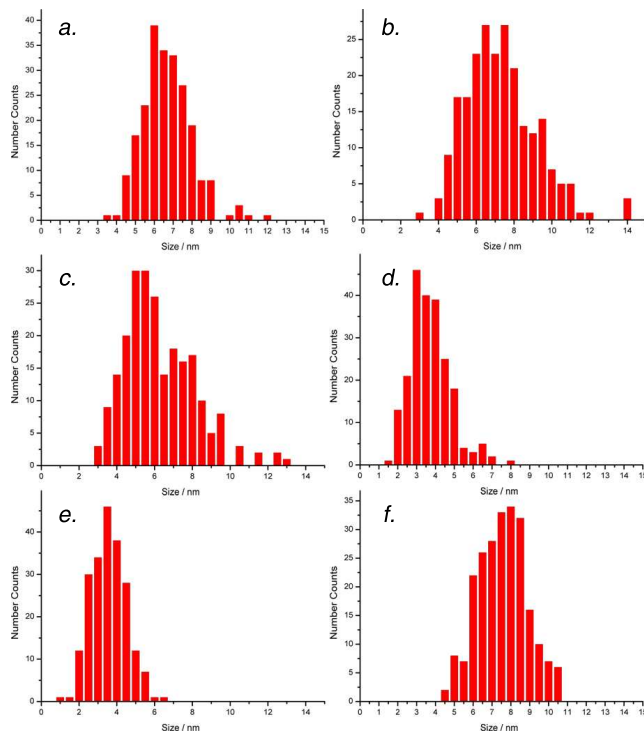
#### Synthesis of cucurbit[5]uril

Synthesis and isolation of cucurbit[5]uril were done according to the reported procedure by Kim *et al.*<sup>1</sup> Isolation and purification of CB[5] were performed according to method reported by our group.<sup>2</sup>

#### Synthesis of gold nanoparticle-capped cucurbit[5]uril composites

A 16 mM stock solution of cucurbit[5]uril (CB[5]) was prepared by dissolving 53.1 mg of CB[5] in 4 mL of deionized water. To 40 mL of 50 % (v / v) aqueous ethanol, an appropriate amount of CB[5] stock solution was added, followed by the addition of an aqueous stock solution of tetrachloroauric acid (20 mM, 0.2 mL, 4 μmol). Sodium borohydride solution (0.1 M in 50 % (v / v) aqueous ethanol, 0.2 mL, 20 μmol) was freshly prepared and added under stirring. The colour of the solution became red, blue, purple and dark red depending on the molar ratio between CB[5] and Au.

## 2 Statistical data of the sizes of AuNPs determined by TEM



**Figure 1:** Histograms of TEM-sizes of CB[5]-AuNP with CB[5]:Au ratio = (a) 0, (b) 0.1, (c) 0.2, (d) 0.5, (e) 1 and (f) from 0 to 1 by addition of CB[5] after the reduction. At least 200 particles were measured for each sample.

**Table 1:** Statistical data on the size and inter-particle distance of AuNP, determined by TEM.

CB[5] : Au	Mean size ± st. dev. / nm	Inter-particle dis- tance ± st. dev. / nm
<b>0</b>	6.5 ± 0.06	Undefined
<b>0.1</b>	7.0 ± 0.10	—
<b>0.2</b>	5.7 ± 0.17	—
<b>0.5</b>	3.5 ± 0.07	—
<b>1</b>	3.5 ± 0.03	0.97 ± 0.02
<b>from 0 to 1</b>	7.6 ± 0.09	0.81 ± 0.02

## References

- (1) J. Kim, I.-S. Jung, S.-Y. Kim, E. Lee, J.-K. Kang, S. Sakamoto, K. Yamaguchi and K. Kim, *J. Am. Chem. Soc.*, 2000, **122**, 540.
- (2) D. Jiao, N. Zhao and O. A. Scherman, *Chem. Commun.*, **2010**, DOI: 10.1039/b920848h.