

Electronic Supplementary Information

Cucurbit[7]uril-stabilized gold nanoparticles as catalysts of nitro compounds reduction reaction

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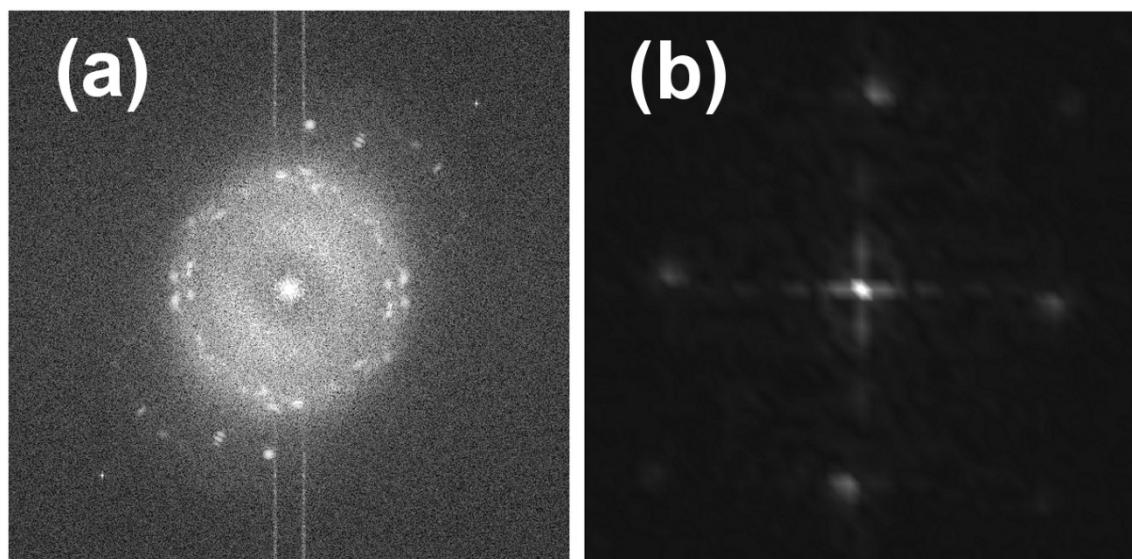


Fig. S1 (a) Selected Area Electron Diffraction (SAED) pattern of a gold nanocrystal. (b) Image obtained after application of 2D-Fast Fourier Transform (2D-FFT) in the marked area of Fig. 1(c).

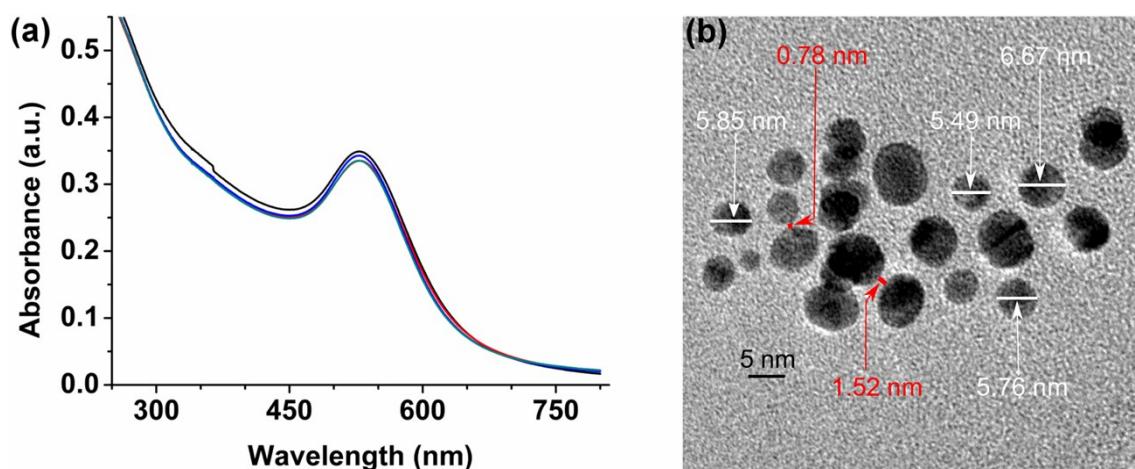


Fig. S2 (a) UV-Vis spectra of the gold suspension just after the synthesis (black) and after 1 (red), 2 (blue) and 3 (green) months. (b) HR-TEM image of 3 months aged AuNPs.

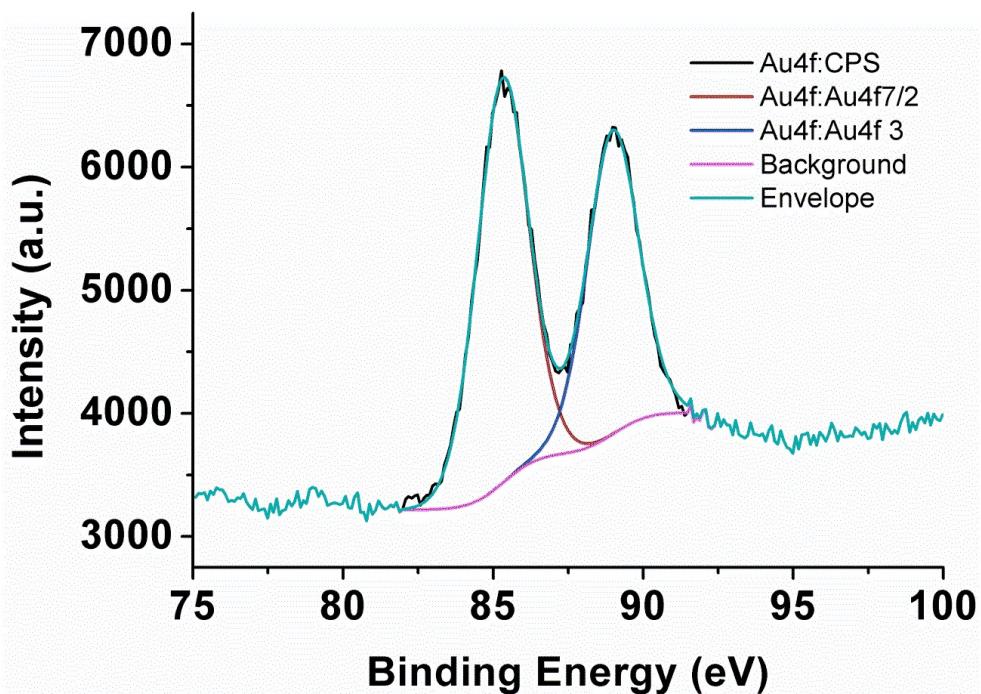


Fig. S3 XPS spectrum of the synthesised AuNPs.

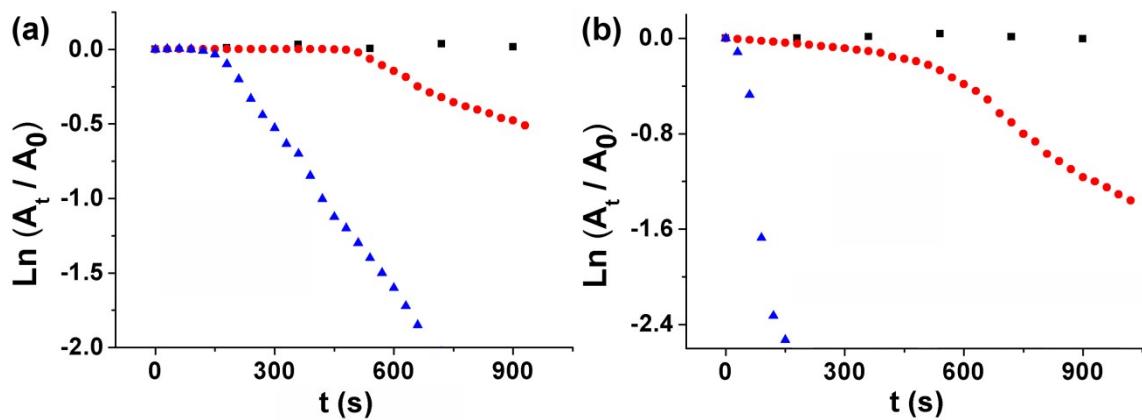


Fig. S4 $\ln(A_t / A_0)$ vs time plots for the reduction of 4-NP (a) and NF (b) at different catalyst volumes: 0 (squares), 25 (circles) and 50 μL (triangles).

Table S1. Comparative table of the apparent kinetic constants obtained for several gold nanosystems (except where indicated) in the 4-NP reduction reaction.

Metal catalyst support or stabilizing agent	T (°C)	NP diameter (nm)	% M(0)/nitro	NaBH ₄ /4-NP	k _{app} (s ⁻¹)	k _{app} (L m ⁻² s ⁻¹)	Ref.
CB7	25	5.7	2.4	100	1.4×10 ⁻³	1.2×10 ⁻¹	1
CB7*	-	2.4	332	44	2.1×10 ⁻²	7.7×10 ⁻³	2
NaBH ₄	-	3.2	0.27	100	9.0×10 ⁻³	3.6×10 ⁻¹	3
1,2,3-triazoles	20	6	0.2	80	1.4×10 ⁻²	4.3×10 ⁻²	4
Mesoporous and oriented boehmite films	25	15-40	280	100	1.7×10 ⁻³	2.7×10 ⁻³	5
Graphene	RT	14.6	45	70	3.2×10 ⁻³	1.9×10 ⁻²	6
Silica nanotubes	RT	3-5	30	42	1.1×10 ⁻²	4.2×10 ⁻²	7
Thermoresponsive micelles	25	3.3	20	33	1.5×10 ⁻³	3.7×10 ⁻³	8
Covalent organic frameworks	RT	5	45	1600	5.4×10 ⁻³	9.7×10 ⁻³	9

*Pd nanoparticles.

Table S2. Induction times for NF and 4-NP reduction reactions in which the reactants order was varied.

Reactants addition order	Induction time (min)
NaBH ₄ + Au + NF	0
NaBH ₄ + Au + 4-NP	≈1.5
NF + Au + NaBH ₄	≈11.0
4-NP + Au + NaBH ₄	≈8.5
NF + NaBH ₄ + Au	≈6.0
4-NP + NaBH ₄ + Au	≈7.5

References

- 1 This work.
- 2 T. Premkumar, K. E. Geckeler, *Mater. Chem. Phys.* **2014**, *148*, 772-777.
- 3 C. Deraedt, L. Salmon, S. Gatard, R. Ciganda, R. Hernandez, J. Ruiz, D. Astruc, *Chem. Commun.* **2014**, *50*, 14194-14196.
- 4 R. Ciganda, N. Li, C. Deraedt, S. Gatard, P. Zhao, L. Salmon, R. Hernandez, J. Ruiz, D. Astruc, *Chem. Commun.* **2014**, *50*, 10126-10129.
- 5 D. Jana, A. Dandapat, G. De, *Langmuir* **2010**, *26*, 12177-12184.
- 6 J. Li, C. Liu, Y. Liu, *J. Mater. Chem.* **2012**, *22*, 8426-8430.
- 7 Z. Zhang, C. Shao, P. Zou, P. Zhang, M. Zhang, J. Mu, Z. Guo, X. Li, C. Wang, Y. Liu, *Chem. Commun.* **2011**, *47*, 3906-3908.
- 8 Y. Wang, G. Wei, W. Zhang, X. Jiang, P. Zheng, L. Shi, A. Dong, *J. Mol. Catal. A: Chem.* **2007**, *266*, 233-238.
- 9 P. Pachfule, S. Kandambeth, D. D. Diaz, R. Banerjee, *Chem. Commun.* **2014**, *50*, 3169-3172.