Electronic supplementary material

Investigation of the role of $NaBH_4$ in the chemical synthesis of gold nanorods

Akshaya K. Samal, Theruvakkattil S. Sreeprasad, Thalappil Pradeep*

DST Unit on Nanoscience (DST UNS), Department of Chemistry and Sophisticated Analytical Instrument Facility, Indian Institute of Technology, Madras, Chennai 600 036 (India)

*Email: pradeep@iitm.ac.in, Fax: 91-44-2257-0545/ 0509.

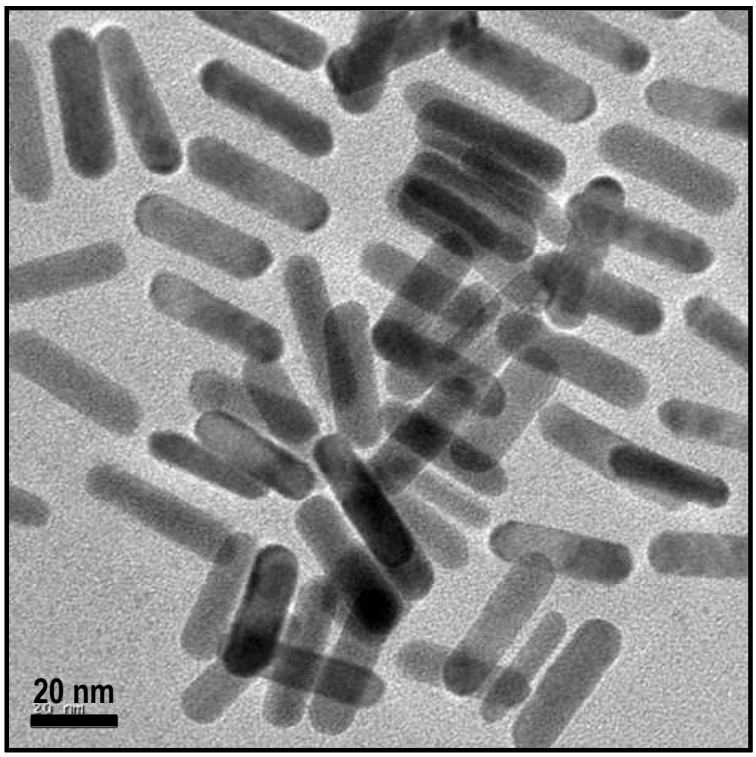

Figure S1. Large area TEM image of GNRs synthesized using Pb seed particles.

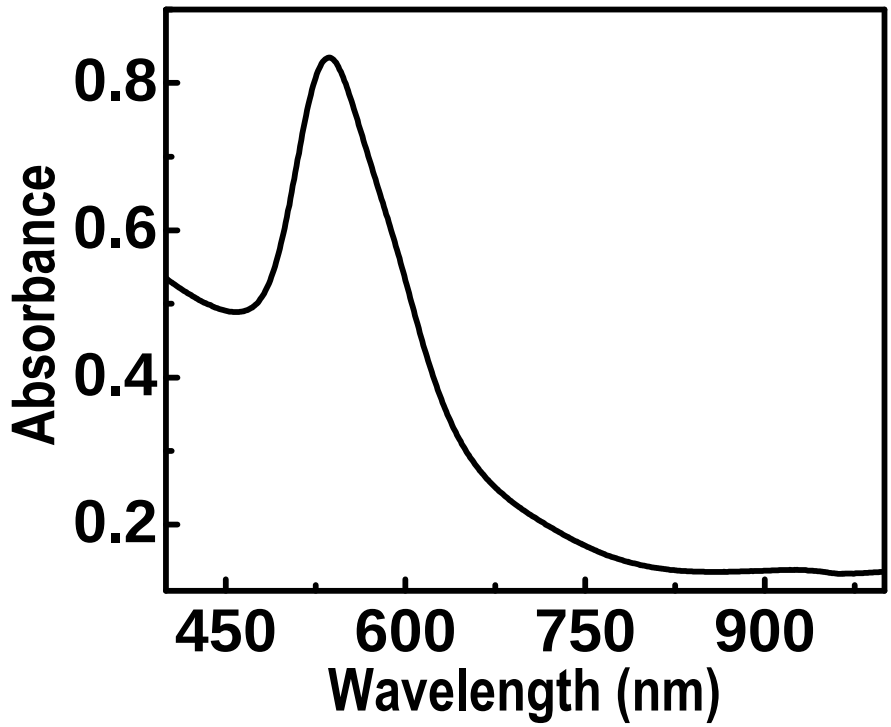

Figure S2. UV-visible spectrum obtained upon the addition of $NaBH_4$ to the growth solution, without silver nitrate.

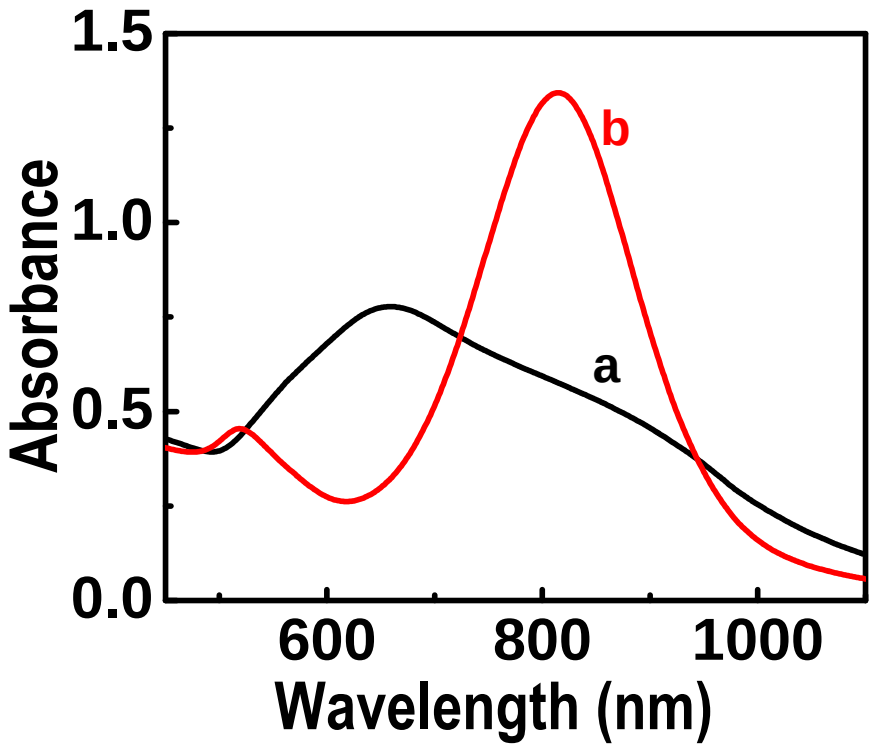

Figure S3. UV-visible spectra of GNRs prepared by using (a) 50 µL of Au@citrate (~16 nm) and (b) 50 µL $NaBH_4$ added Au@citrate (100 µL $NaBH_4$ was added to 500 µL of Au@citrate and from this 50 µL $NaBH_4$ added to the growth solution). Various shapes were observed in TEM for trace a.

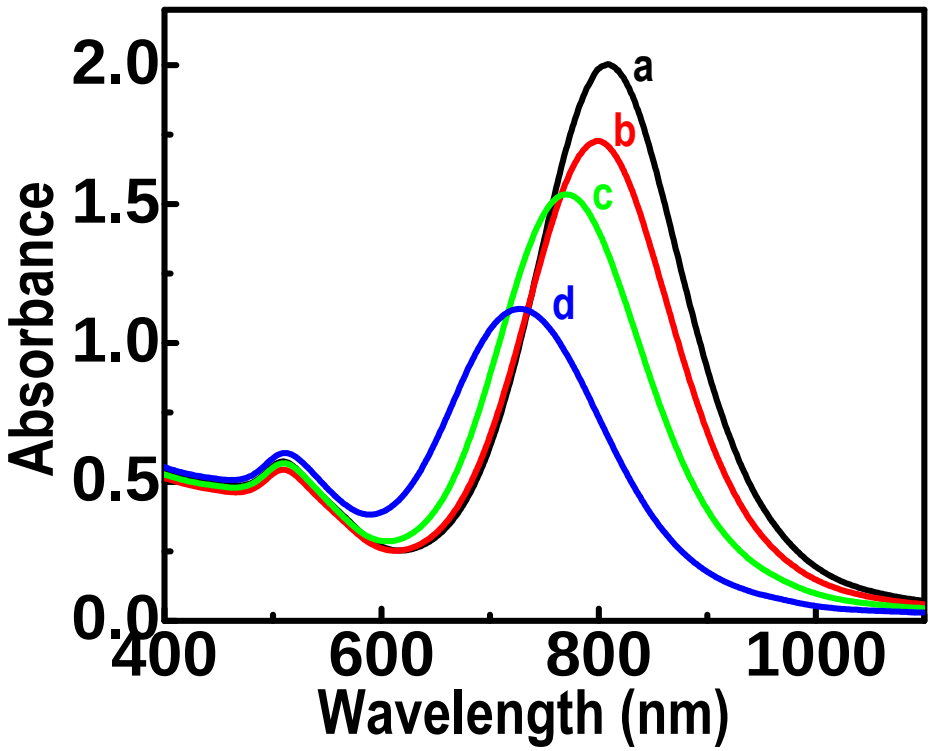

Figure S4. UV-visible spectra of GNRs formed with increasing amount of seed solution; (a) 105 µL, (b) 210 µL, (c) 420 µL, and (d) 630 µL.

S5. Determination of effective BH_4^- (or electrons) used in the GNR formation

The following calculations illustrate two important aspects:

1. Some of the Au^{1+} undergoes reduction to $Au^{(0)}$ initially forming in-situ seeds. The remaining Au^{1+} ions get reduced on the preferred surfaces of the seeds, forming GNRs.

2. The effective moles/number of electrons available for the reduction of Au^{1+} has a strong similarity in the two methods of GNR formation (seed-mediated synthesis and direct addition of $NaBH_4$ to the growth solution).

Seed-mediated growth of GNRs:

Composition of the seed solution:

CTAB: 100 mM, 7.5 ml

Au^{3+}: 10 mM, 250 µl → Number of moles of Au^{3+} = 2.5 µmoles

$NaBH_4$: 10 mM, 600 µl → Number of moles of BH_4^- = 6 µmoles

3 moles of BH_4^- will reduce 8 moles of Au^{3+} to $Au^{(0)}$ in the seed solution

[Note: $BH_4^- + 3H_2O \rightarrow B(OH)_3 + 7H^+ + 8e^-$

$AuCl_4^- + 3e^- \rightarrow Au^{(0)} + 4Cl^-$]

1 mole of Au^{3+} need to be reduced = 3/8 moles BH_4^-

2.5 µmoles of Au^{3+} need to be reduced = 2.5 * 3/8 = 0.9375 µmoles BH_4^-

Remaining BH_4^- present in the seed solution = 6 - 0.9375 = 5.0625 µmoles

Total volume of seed solution prepared = 8350 µl

Seed solution added to growth = 105 µl

Effective moles of BH_4^- added through seeds = 105/8350 * 5.0625 = 0.0636 µmoles

Number of moles of electrons added through seeds to the growth solution = 0.0636*8 = 0.5088 µmoles

$NaBH_4$ assisted *in-situ* growth of GNRs:

50 µl, 1.67 mM $NaBH_4$ was added to the growth solution

Effective moles of BH_4^- added = 1.67*50 = 0.0835 µmoles

Number of moles of electrons added to the growth solution = 0.0835*8 = 0.668 µmoles

Effective BH_4^- (in µmoles) was calculated similarly in all cases. This was used to make Figure 9.

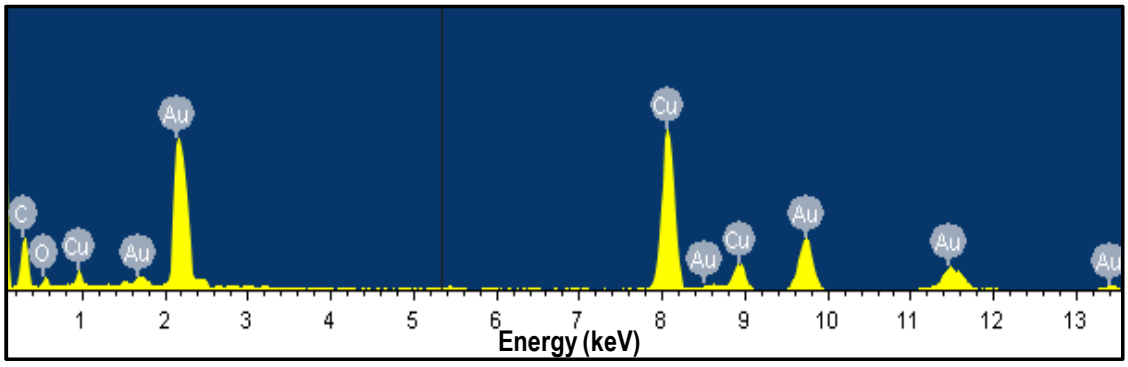

Figure S6. EDAX spectrum of GNRs synthesized using Pb seed particles. The presence of Cu is due to the copper grid used.