# Molecular charge transport : relating orbital structures to the conductance properties

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# A

# How to synthesize superior gold nanoparticles

## A.1 Ingredients

Serves 100 ml gold nanoparticles in water with approximatelly $10^{13}$ particles.ml$^{-1}$ (stock solution). To transfer the nanoparticles to a chloroform solution we use 10 centrifuge tubes of 1 ml. Takes $\approx \frac{1}{2}$ day.

- 79 ml ultra-pure water (18.2 $\Omega.m^{-1}$)
- 1 ml $HAuCl_4$ solution (1% weight/volume in ultra-pure water)
- 80 $\mu$l tannic acid solution (1% weight/volume in ultra-pure water)
- 4 ml trisodium citrate (1% weight/volume in ultra-pure water)
- 16 ml ultra-pure water
- 0.194 ml octanethiol
- 22 ml ethanol (Ar flushed)
- 8 ml chloroform

- 2 Erlenmeyer
- 1 magnetic stirrer
- 1 heating plate with magnetic stirrer
- 10 eppendorf centrifuge tubes (2 ml)
- 1 centrifuge
- 1 water-cooled ultrasonic bath
- 1 glass vial
- water-cooled reflux
- nitrogen flushed glove box

## A.2 Gold nanoparticles in water

- In one Erlenmeyer mix the $HAuCl_4$ solution with the 79 ml water and heat up to 60° C on the heating plate.
- In the other Erlenmeyer mix the tannic acid, the trisodium citrate and the 16 ml water and heat as well up to 60° C on the heating plate.
- When both solutions are at 60° C, mix the two solution using the magnetic stirrer and bring to boiling point with the reflux connected.
- Keep boiling for 10 minutes. The solution will turn from blue purple to rubby red.
- Let the solution cool down to RT while stirring.
- This solution of nanoparticles in water is stable for month in the refrigerator.

## A.3 Gold nanoparticles in chloroform

- Divide 20 ml gold NP solution into 10 centrifuge tubes
- Centrifuge for 60 minutes, at 10 ° C at 15000 rpm
- While centrifuging make the octanethiol solution in ethanol (0.14 M). Mix 0.194 ml octanethiol in 8 ml ethanol in the glove box.

- Remove the suppernattant (water) from the centrifuge tubes.
- Add 1.5 ml ethanol (nitrogen flushed) into each tube and shake.
- Collect the solution from all the tubes into a glass vial. Put in the ultrasonic bath for 10 seconds.
- Add the octanethiol solution to the vial at once. Put in the ultrasonic bath for 10 seconds. Keep in refrigerator for at least 2 days.
- Once the nanoparticles are sedimented (black residue on the bottom of the vial), remove the ethanol and replace with the chloroform. Put in the cooled ultrasonic bath for 1 hour (recovered ruby red colour).
- The nanoparticles are ready to use, enjoy!