Title: **Shaped silver nanoparticles for direct plasmonic solar cell application**

Student: Alba Gascón Nicolás

Date: June 2020

Supervisor/s: Prof. Jacinto Sá
Departament of Chemistry
Uppsala University

Solar cells have a pivotal role in solving the problem of climate change. Since the first reported device, in 1946, up to four generations of cells have been described. The current generation consists of organic, perovskite and plasmonic solar cells. The group of Prof. Jacinto Sá pioneered the concept of ultra-thin transparent solid-state plasmonic solar cells, using silver as light absorber. Currently, the cell produces 20 µA/cm2 and 0.8 V, using silver nanoparticles absorbing between 300-500 nm. To improve the solar cell performance without affecting overall transparency, one must expand light absorption from 500-900 nm. Two strategies can be followed to achieve this, namely changing the size or the shape of the particles. Increasing the size will make the particles to absorb more in the visible region but large particles have lower absorption coefficients and reduce surface area limiting charge transfer. Shaping the particles, i.e. producing for example prisms instead of spheres, shifts equally the absorption without compromising the surface area and light absorption.

The aim of the present project was to prepare and modify silver nanoprisms particles and study their characteristics and stability. Three different samples, SA, SB and SC, have been produced following a two-step synthetic procedure. They have been chosen in order to fit the objective concerning the expand of light absorption. Figure 1 shows how by mixing tuning the

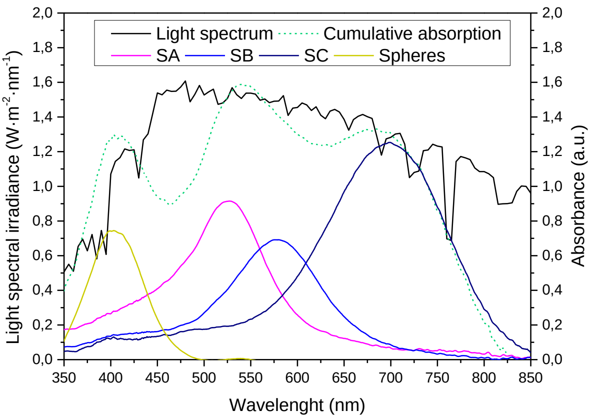

Figure 1 Light spectral irradiance and silver nanoparticles UV-Vis absorption spectra.

concentration of individual samples one can match the light spectrum. This ability would applly to match any type of illumination that the cell will be exposed to (outdoor and indoor).

Two main parts are presented: the study of the particles and their modification with a linker molecule. Firstly, is important to deeply understand which are the parameters that suit the most the synthesis and the storage conditions. Secondly, a linker molecule is needed to anchor the metallic particles as well as to prevent the Fermi levels of the semiconductor and the metallic nanoparticles to equilibrate and therefore to lose the Schottky barrier. The dipole characteristic of the molecule promotes charge injection and its pie benzene ring, flat and rigid, facilitates the electron transfer. To build a solar cell one of the strategies followed is building layer by layer. Achieving a stable mitxture of metallic nanoparticles and linker is crucial to speed up the process, saving one step.

In the first part, reproducibility, purification and stability studies have been perfomed. Reproducibility is studied by comparing the characteristics of different lots of samples synthesized. The purification is assessed by assuring that the sample is not damaged after the centrifuging process. For the stability, two studies are performed, one consists on tracking the characteristics of a sample through different days. The other one is a test performed with sodium chloride, in which the samples are damaged by adding small quantities of an aqueous solution of the salt, the stabler the sample, the slower the damage will result, i.e. more additions will be needed. The results show that the followed methods are reproducible to the extent that the application demands. That samples can be purified, although they show more stability if they are kept as prepared. Finally, noticeable changes appear in the particles during the two first days after they have been synthesized, and after this amount of time, important changes are only observed when comparing measurements performed in time ranges of more than 4 days.

The second part is introduced with a spectroscopic study, SERS, performed on silver nanospheres that proves the linking configuration between 4-aminobenzoic acid (PABA), the linker used, and the metallic nanoparticles. It follows with threshold value studies, where the guiding values of the highests concentrations of PABA that do not damage the samples are given. Finally, the stability studies, using NaCl tests, reveal that particles are more stable when stored alone. Furthermore, the results show that the hypothesis, which says that the linker substitutes the capping agent, is the most plausible one.