Morphological transitions of CTAB aggregates

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More than 150 years ago, Faraday discovered some peculiar properties of the colloids, in particular gold colloids ("Gold becomes partially transparent not as a result of cracks or holes, but by the brightness of the light through their environment"). Today, thanks to the rise of nanotechnology, numerous synthesis methods of gold colloids have been developed during the last years, and got multitude of applications.

One of the most common synthesis methods is the growth from gold seeds that autocatalyze the reduction of gold ions on the surface of the seed. In this method, the use of some surfactant that prevents gold seeds from being added and controls the morphology of the colloids formed. This is because the surfactant is added around the seeds and controls the flow to the surface of gold salts. Depending on the concentration of surfactant used in the synthesis are able to generate channels of water on the surface of the seed. These channels allow a optimal heat transfer between the water at the same time that allow a reformation of the seeds that like result they generate perfect nanoparticles from an optical point of view, as is the case of the nanorods.

To try to understand the details of this mechanism we performed Molecular Dynamics (MD) simulations for a different number of CTAB molecules present in the aggregates at different concentrations of a widely used surfactant such as CTAB. In our work we have found several morphological transitions for the CTAB in dissolution, ranging from micelles to bilayers or perfectlys developed cylinders.

On the other hand we have seen that the surfactant is added forming micelles on the surface of gold whose internal structure depends on the surface golden atom on which it is adsorbed. MD simulations have helped us to understand this mechanism by providing a microscopic explanation about the growth of gold nanorods and thereby try to optimize the synthesis processes with the the aim of making them more efficient.

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