Influence of Cd-to-S and Cd-to-MAA molar ratios in the size and photoluminescence properties of CdS QDs synthesized in aqueous medium

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Among the many experimental variables affecting the stability, dispersion and photoluminescence properties of CdS nanoparticles synthesized in aqueous medium, the molar ratio of the species forming NPs is of great importance.

In order to choose the optimum molar ratios of the species involved, we carried out two types of experiments: on the one hand we studied the effect of the concentration of the dispersant agent (MAA, mercaptoacetic acid), keeping constant Cd-to-S ratio and, on the other hand we investigated the effect of the change of Cd-to-S ratio maintaining Cd-to-MAA ratio constant.

Experimental results obtained show that the environment in which the nanoparticles are formed is important in the processes of nucleation and growth and in the state and shape of the nanoparticle surface. The nucleation process does not merely involve the approach of Cd^{2+} y S^{2-} ions; Cd/MAA ions may also be involved and because of it the kinetics in the process of synthesis of nanoparticles may depend on the concentration of the dispersant agent. From a practical point of view the most fluorescent nanoparticles were obtained for a Cd-to-MAA ratio in the range 1:2. Moreover, our work demonstrates the need to have excess of cadmium in the synthesis of our NPs for the formation of a *nanoshell* of $Cd(OH)_2$, which directly affects the fluorescence intensity. The highest fluorescence intensity would be achieved for an optimum ratio between the thickness of the nanoshell and the mean diameter of the NPs. If the nanoshell is a very narrow deposit with regard to the mean diameter, only the transfer of electrons through it is improved, increasing slightly the quantum efficiency in the excitation-emission process. When the nanoshell is large regarding the nanoparticle diameter, the transfer of electrons through it in the excitation process increases but during the emission process the non-radiant energy fraction is increased. The intermediate situation, with an optimum ratio between nanoshell width and mean particle diameter affords the highest quantum efficiency.