

# OPTICAL CHARACTERISTICS AND HIGH RESOLUTION 2D DOSY NMR IN CdSe QUANTUM DOTS

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Semiconductor quantum dots (QDs) attracted extensive research efforts over the last decade because of their potential for various applications in optoelectronics, photonics, medicine, etc. In spite of the problems related to the toxicity of Cd compounds, the possibility of tuning of the optical parameters of CdSe QDs makes them very attractive for technological development as well as for optoelectronics and biomedical applications [1].

We present experimental results on preparation and characterization of colloidal CdSe QDs in organic solvent. Colloidal semiconductor QDs were prepared via a chemical route. Typically the synthesis of the nanocrystals CdSe was carried out at 170 °C. Different sized QDs were obtained by varying the reaction time. The colloidal quantum dots solutions were collected at determined reaction time interval after the injection for obtaining the desired size of quantum dots. The obtained CdSe QDs were isolated and purified by adding acetone to the cooled solution followed by centrifugation at 8000 rpm for about 30 min. CdSe nanoparticles have been characterized by UV-Vis absorption and photoluminescent (PL) spectroscopy as well as by 2D diffusion-ordered nuclear magnetic resonance spectroscopy (2D DOSY NMR). The average CdSe particles size for three selected samples was estimated from the position of the first excitonic peak [2,3] in the UV-Vis absorption spectrum and was found to be in the range 2.28 - 2.92 nm which correlates very well with the results obtained from high resolution 2D DOSY NMR. NMR was measured in the conditions of Z gradient strength 5.57 G/cmA, gradient pulse 1 ms and delay for gradient recovery 0.1 ms. The CdSe QDs sizes were determined on the basis of diffusion-ordered <sup>1</sup>H spectra related to one- or two-molecular layers of oleic acid covering QDs. In high resolution 2D DOSY NMR, even modest differences in diffusion coefficient between species are sufficient to allow the spectrum of an intact mixture to be decomposed into sub-spectra of individual components. PL spectra were measured under excitation of a laser beam 337 or 405 nm using a MDR-23 monochromator and a photon counting module H9319-12 connected to a PC. The absorbance spectra of the colloidal chloroform solutions of CdSe QDs have been registered in the range 300-800 nm. The absorption peaks appear very clear on each curve, indicating the presence of CdSe QDs. The reaction time for selected samples was increased by 50 s, and the absorption peak red-shifts from 494.7 up to 543 nm, sequentially. The absorption edge is relatively sharp, indicating a relatively narrow size distribution of the nanoparticles. The PL spectra for CdSe nanodots can be characterized by the presence of a main almost Gaussian-shaped line with the peak maximum shifting from 508 nm to 566 nm in dependence of the CdSe nanoparticle size. The PL emission spectra of CdSe QDs is dominated by a near-band-edge emission, while a weak broad band in the 600-800 nm range, related to the surface shallow trap emission is markedly suppressed. The PL spectrum can be deconvoluted in a major Gaussian line, positioned at 508 nm, and other two low intensities bands shifted toward red wavelengths. While the CdSe QDs size tends to increase with increasing the reaction time, the PL bands shifts from 508 to 566 nm, which correlates with the position of the main excitonic peak shifting in the absorption spectrum. The small line width of the main PL band suggests that particles have a narrow size distribution, while the low intensity emission from surface trap states at longer wavelengths suggests low concentration of surface defects.

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