Nanocomposites and nanomaterials

Optical and electrochemical monitoring of band structure of Hg-alloyed CdTe colloidal QDs.

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The near-infrared $Cd_{1-x}Hg_xTe$ QDs are the most studied CdTe based semiconductor nanocomposites which are widely used for biological imaging, solar cells and telecommunication. Thus, it is important to understand the effects of alloying on the band structure of CdTe QDs.

The series of thioglycolic acid-stabilized colloidal $Cd_{1-x}Hg_xTe$ QDs ($d \approx 2.3$ nm) with different Hg^{2+} content were prepared in water solution by an ion-exchange reaction. The resulting samples were characterized using UV-vis absorption and photoluminescent (PL) optical spectroscopic studies, cyclic voltammetry (CV) and scanning transmission electron microscopy (STEM).

We observed red-shift of the PL peaks to the near-infrared region of the spectrum from 538 to 902 nm depending on the Hg^{2+} content. It should be noted, that occurrence of double-peak and triple-peak structures of PL spectra takes place. Based on the CV data, we can assert that the reason of such evolution of the PL spectra is caused by gradual transformation of CdTe QDs band structure during the Hg-alloying process. We propose three-stage scheme of CdTe QDs modification by Hg-alloying:

$$\text{CdTe QDs} \xrightarrow[+Hg^{2+}]{-Cd^{2+}} \text{CdTe/ } Cd_{1-x}Hg_xTe \text{ QDs} \xrightarrow[+Hg^{2+}]{-Cd^{2+}} \text{CdTe/ } Cd_{1-x}Hg_xTe \text{/HgTe QDs} \xrightarrow[+Hg^{2+}]{-Cd^{2+}} Cd_{1-x}Hg_xTe \text{/HgTe QDs}$$

In general, increasing concentration of Hg^{2+} in $Cd_{1-x}Hg_xTe$ QDs leads to a decrease in band gap energy as the result of the significant difference between the band gap energies of CdTe and HgTe [1]. Such alteration of $Cd_{1-x}Hg_xTe$ QDs band structure are caused by the generation of new energy levels. Based on the obtained results, we propose the energy level diagram of CdTe and $Cd_{1-x}Hg_xTe$ QDs.

1. *Smith A., Lane L., Nie S.* Mapping the spatial distribution of charge carriers in quantum-confined heterostructures // Nature communications.-2014.- **5**-P. 4506-4518