THE EFFECTS OF EMBEDDING MEDIUM AND SIZE ON OPTICAL PROPERTIES OF II-VI CORE/SHELL NANOCRYSTALS

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Recently, a family of water-soluble quantum dots (QDs) that exhibit low nonspecific binding to cells, small hydrodynamic diameter, tunable surface charge, high quantum yield, and good solution stability across wide range of pH has been reported [1]. The choice of these high-yield QDs is based on their sizes, optical properties and toxicity. For imaging applications, the QD emission wavelength should ideally be in a region of the spectrum where blood and tissue absorb minimally but detectors are still efficient (approximately 700-900 nm) in the near-infrared. In addition, the hydrodynamic size of the QD should be appropriately matched to the biological molecules. To find good fluorescent labels for biological macromolecules, II-VI quantum dots enclosed in a II-VI semiconductor shell and both surrounded by organic or inorganic medium have been developed for a large number of applications (see for example ref. [2]).
The aim of this work is to investigate the optical properties (absorption, scattering and extinction) of II-VI core/shell nanostructures in a wide range of visible and near-infrared spectrum of light. In dipole approximation, the Mie scattering theory is applied to nanoshell systems to calculate the absorption, scattering and extinction coefficients [3]. To implement the calculations, Mie theory requires the dielectric function to be clearly defined. So, in this work an explicit expression of frequency-dielectric function for both the core and shell is used and it includes the phonon and plasmon contributions as defined in reference [4] i.e.,

$$\varepsilon_i(\omega)=\varepsilon_i(\infty)\left[1+\frac{\omega_{LO,i}^2-\omega_{TO,i}^2}{\omega_{TO,i}^2-\omega^2-i\gamma_i\omega}-\frac{\omega_{p,i}^2}{\omega^2+i\gamma_{p,i}\omega}\right] \qquad (i=1,2). \qquad (1)$$

In eq. (1), $\varepsilon_i(\infty)$ are the high-frequency dielectric constants of core (1) and shell (2) respectively; $\omega_{TO,i}$ and $\omega_{LO,i}$ the transverse and longitudinal frequencies of the polar modes and γ_i their damping constants; $\omega_{p,i}$ and $\gamma_{p,i}$ are respectively the frequencies and the damping constants of the plasmons for core and shell materials.
The system under investigation is described in figure 1 with its respective geometric sizes. Core and shell are embedded by an insulating medium with dielectric constant ε_3 (see figure 1).
Effects of shell-size and insulating media on the optical properties are investigated. As an example, we show in figure 2 the scattering coefficient of CdS/ZnS/glass nanoshell as a function of the wavelength for three different sizes of the shell. Clearly, the scattering coefficient is greater for increasing size of core/shell nanostructure and it decreases for increasing wavelength as it is predicted by experiments.

References:

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Figures:

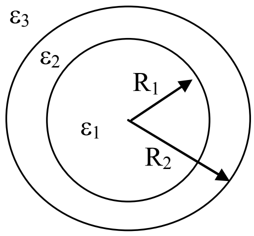

Figure 1: Scheme of a core/shell nanocrystal: ε_1 and ε_2 are frequency-dependent dielectric functions of the core and shell, R_1 and R_2 their respective radii .

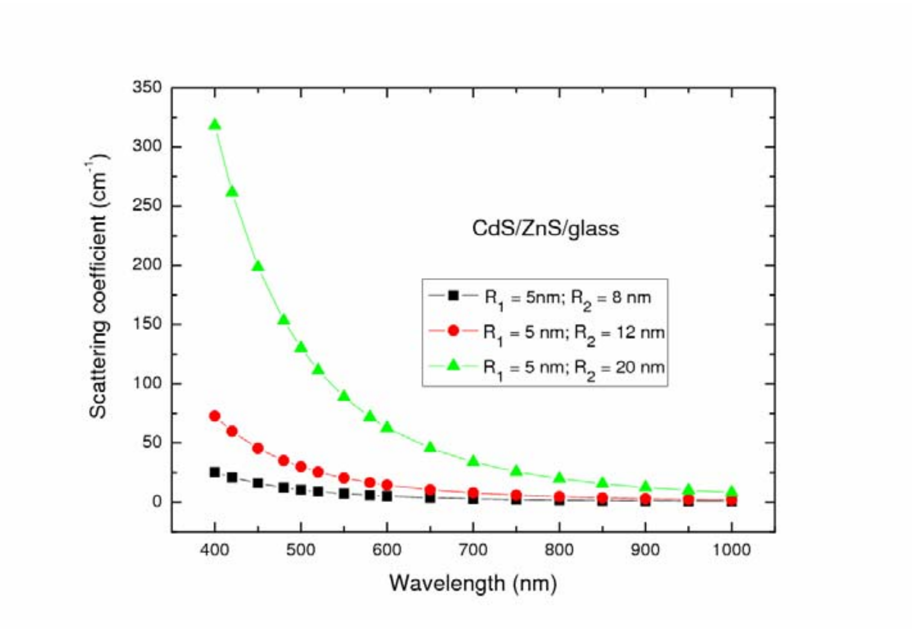

Figure 2: Scattering coefficient of CdS/ZnS/glass nanoshell versus λ (wavelength) for different values of shell-sizes.