Synthesis, Surface Functionalization, and Biological Sensing Applications of Compound Semiconductor Nanocrystals

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Abstract

Nanocrystals of II-VI compound semiconductors, such as CdSe and ZnSe, have unique properties, including size-tunable photoluminescence, narrow emission and broad absorption spectra, high quantum yields, large extinction coefficients, and excellent photochemical stability. These materials are being studied as potential candidates for a wide range of novel applications in medical diagnostics, display technologies, and solar energy conversion. ZnSe nanocrystals are particularly attractive, because they do not contain toxic heavy metal ions, such as Cd^{2+}, and can be easily doped with transition metal ions, thus providing additional control over their electronic properties. We have developed a novel technique for the synthesis of compound semiconductor nanocrystals by employing microemulsions and liquid crystals as templates to precisely control the size and shape of the nanocrystals. Stochastic simulations of the process were performed to investigate the underlying mechanisms and scaling laws of particle nucleation and growth were extracted. Density functional theory calculations elucidated the doping mechanisms and the thermodynamic stability of core-shell structures. Extraction of the nanocrystals from the growth media and functionalization of their surface with organic bi-functional molecules has enabled their stabilization in aqueous solutions and subsequent conjugation with probe biomolecules. A new class of optical biosensors has been developed based on biomolecular probes bound to ZnSe nanocrystals that enable rapid quantitative detection of biological targets. Binding of the biosensors to target biomolecules changes the fluorescence emission spectrum of the ZnSe nanocrystals, thus producing an optical signal that can be detected without prior separation of the sensor-target complex. Detection of single-base DNA mutations and separation-free assays, that enable rapid quantitative detection of proteins in solution, have been demonstrated. The new biosensors are suitable for developing portable devices that can provide rapid multiplexed detection of biological targets for point-of-care diagnostic applications.