

Biologically Programmed Synthesis of Core-Shell CdSe/ZnS Nanocrystals

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Supporting Information

Experimental Procedure

Bi-functional peptide:

Bi-functional peptide was chemically synthesized by American Peptide Company (Sunnyvale, CA). The CdSe formation domain was –Cys-Thr-Tyr-Ser-Arg-Lys-His-Lys-Cys- (Cys-Cys Disulfide Bridge) while ZnS domain was -Lys-Arg-Arg-Ser-Ser-Glu-Ala-His-Asn-Ser-Ile-Val-. The two domains were linked via Proline.

Nanocrystal synthesis:

For CdSe synthesis 5mM CdCl₂ was mixed with 20μM bi-functional peptide and rotated at room temperature for 1.5 hours under oxygen free environment. Thereafter 2.5mM freshly prepared NaHSe was added to CdCl₂-peptide solution at pH 11 to a final volume of 400 μL. NaHSe was prepared according to reference 25; briefly 80 mg NaBH₄, was transferred into 1 ml water and 80 mg selenium powder was added. The tube was placed on ice and capped by paraffin with a small pin hole to allow pressure release built by hydrogen production. Selenium powder disappeared in about 30 min, and white crystals appeared which were diluted in oxygen free water to make 25mM NaHSe stock solution. NaHSe-CdCl₂-peptide solution was further allowed to react for 1.5 hours and heated at 95°C for 30 minutes. Such produced CdSe solution was dialyzed to get rid of free reactants.

Synthesis of ZnS was performed in a similar way; where 1mM ZnCl₂ was incubated with 20μM bi-functional peptide and rotated at room temperature for 1.5 hours. Freshly prepared 1mM Na₂S was added to the solution and rotated for another 1.5 hours and heated at 95°C for 30 min. To synthesize CdSe/ZnS nanoparticles, CdSe nanoparticles were synthesized as described previously and were used as the starting material for ZnS shell growth. 200μL of these CdSe particles was allowed to interact with 0.5mM ZnCl₂ for 1.5 hours and then 20μM bi-functional peptide was added to react with the solution for another 1.5 hours. Separate reactions were also run with 0.5mM ZnCl₂ and 20μM bi-functional peptide only. To both the solutions 0.5mM Na₂S was added and reacted for 1.5 hours followed by 30 min heating at 95°C. The particles were purified using dialysis as described previously.

Characterization:

UV-visible transmission spectra were obtained using a Shimadzu 3100 UV-Vis-NIR spectrophotometer. Photoluminescence measurements were done using Shimadzu RF-5301 PC spectrofluorometer. All optical measurements were performed at room temperature under environmental conditions.

For TEM and HRTEM 10μL of nanoparticle solution was dropped on a carbon-coated 400-mesh copper grid and dried under an incandescent lamp. TEM and HRTEM were performed with a FEI CM300 high resolution transmission electron microscope operated at an accelerating voltage of 300 kV. HRTEM lattice imaging and electron diffraction were used to determine the crystal structures.

Elemental analysis was performed by energy dispersive X-ray spectroscopy (EDXS) for the presence of various relevant elements. The cadmium peaks from K and L shells were

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observed at ~23keV and ~3keV, respectively. Selenide (at ~2KeV & 11KeV), Zinc (at ~8.5keV), and Sulfide (at ~2.5KeV) peaks were observed for CdSe/ZnS nanoparticles. A copper peak by TEM copper grid was detected at ~8KeV.

Fig. S1 Photoluminescence (excitation at 410 nm) of the synthesized CdSe and core-shell CdSe-ZnS nanocrystals

