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Supplementary data

Transparent conducting films of CdSe(ZnS) core(shell) quantum dot (QD) xerogels

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Experimental Details

Materials

Selenium powder (99.5%), diethylzinc (1M, in hexane), Bis(trimethylsilyl)sulfide, trioctylphosphine oxide (TOPO, 90%), tetranitromethane (TNM), and 11-mercaptoundecanoic acid (MUA, 95%) were purchased from Aldrich. Trioctylphosphine (TOP, 97%) and cadmium oxide (99.999%) were purchased from Strem Chemicals. 1-tetradecylphosphonic acid (TDPA, 98%) was purchased from Alfa-Aesar and tetramethylammonium hydroxide pentahydrate (TMAH, 97%) was purchased from ACROS. Toluene, methanol, and ethyl acetate were purchased from Mallinckrodt. TOPO was distilled before use; all other chemicals were used as received.

Synthesis of CdSe and CdSe(ZnS) QDs

CdSe(ZnS) core(shell) QDs were synthesized according to literature methods with slight modifications.[1,2] In a typical synthesis of QDs, a mixture of 0.0127 g (0.1 mmol) of cadmium oxide, 0.04 g (0.14 mmol) of 1-tetradecylphosphonic acid and 2.0 g (5.17 mmol) of trioctylphosphine oxide were heated to 330 ˚C under argon flow. After the solution became colorless, the temperature was reduced to 150 ˚C and a solution of selenium containing 0.01 g (0.13 mmol) of selenium powder in 2.4 mL of trioctylphosphine was injected. The temperature of the mixture was then increased up to 250 ˚C at a rate of 10 ˚C per 10 minutes and the QDs were grown for four hours.

A mixture of 0.15 mL of 1M diethyl zinc in hexane, 0.03 mL of bis(trimethylsilyl)sulfide (0.14 mmol) and 2 ml of trioctylphosphine was slowly injected over a time period of 15 minutes (the total molar ratio of the injection solution targeted CdSe:ZnS 1:1.4) using a syringe pump at 180 ˚C to synthesize the ZnS shell, and core(shell) QDs were annealed at 75 ˚C overnight. As-prepared CdSe(ZnS) core(shell) QDs were purified by two cycles of dispersion in toluene and precipitation with methanol.

MUA exchange

0.3678g (1.6 mmol) of MUA was dissolved in 10 mL of methanol and the pH increased up to ~ 10 using TMAH. QDs were dispersed in MUA solution (Cd:MUA molar ratio of 1: 4, based on original moles of Cd employed in the synthesis) and centrifuged to remove the original organic ligands. The QDs were washed with ethyl acetate to remove excess MUA ligands and dispersed in methanol to make QD sols.

Deposition of CdSe(ZnS) xerogel films by sol-gel methods

Glass slides (Becton, Dickinson and Co.) were used as substrates for film deposition. Slides were cut to 1 cm by 1 cm and sonicated in acetone and ethanol, respectively, for 15 minutes. After rinsing with distilled water, the glass slides were dried under nitrogen gas blow. For the film deposition, glass slides were immersed in different volumes (ranging from 3 mL to 5 mL, particle concentration of 4 x 10^{-7} M) of pre-oxidized MUA-capped CdSe(ZnS) sols in compartmentalized Petri dishes (4 sections, 100mm (diameter) x 15mm (height), Fisher Scientific). 10 μL of TNM was then added to oxidize the MUA ligands, resulting in aggregation. After gelation, the substrates were dipped in acetone to remove the gelation by-products and dried under ambient conditions to make xerogel films.

<u>Characterization of films</u>

X-ray diffraction (XRD)

XRD was performed on a Rigaku Diffractometer (RU200B) using the Kα line of a Cu rotating anode source (40 kV, 150 mA).

PL and UV-vis spectroscopy

PL and UV-vis spectra were obtained with a Cary Eclipse (Varian, Inc.) fluorescence spectrometer and a Cary 50 (Varian, Inc.) spectrophotometer, respectively.

Field emission scanning electron microscopy (FESEM)

FESEM images were obtained using a JEOL JSM-7600F field emission scanning electron microscope operated at an accelerating voltage of 15 kV in high-vacuum mode. The glass substrate-supported films were coated with a thin layer of gold by sputtering. EDS spectra were recorded using an EDAX detector installed on the FESEM.

Atomic force microscopy (AFM)

AFM was performed using a Dimension 3100 AFM (VEECO) in tapping mode. The surface roughness was measured by using the roughness command (Nanoscope) from three areas of 5×5 μm^2 size on the film. Then the film was scratched carefully with a blade. The film thickness was determined using the sectional height analysis command (Nanoscope) by measuring the depth of the scratch at five locations on the film.

Sheet resistance measurements

Sheet resistances of the deposited films were measured using the van der Pauw method with a Keithley 2400 source meter. Four Pt wires and silver paste were used to achieve ohmic contact with the film, defining approximately a square of 1 cm^2.[3]

References

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