Blue emitting Copper doped Zinc Oxide nanocrystals

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Supporting Data:

(a) Synthesis of Cu doped ZnO:

The synthesis of Cu doped ZnO nanocrystals was carried out in solution using isopropanol as a solvent. A typical synthesis involves dissolving the required stoichiometric percentage of 0.5 mmol of copper acetate in 0.5 mL of water and added to 100 mL of isopropanol with constant stirring. To this solution, the residual percentage of 0.5 mmol of zinc acetate was added with constant stirring at 50 °C. Then 0.3 mmol of poly-vinyl pyrrolidone (PVP) (Molecular weight ~ 10,000) was added under continued stirring. PVP was not added for the synthesis of free standing nanocrystals. This solution was hydrolyzed by 1.25 mmol solution of NaOH in 50 mL of isopropanol under ultrasonic agitation for two hours and then the solvent was removed by rotavaporization. The particles were washed in water, centrifuged and then dried in vacuum for 8 hours.

(b) Characterization of Cu doped ZnO:

The size of the particles were determined from TEM images obtained using JEM 2010 HRTEM, JEOL microscope at an accelerating voltage of 200 keV. Samples for TEM were prepared by making a clear dispersion of the nanocrystals in i-PrOH and putting a drop of the solution on a carbon coated copper grid. The solution was allowed to evaporate leaving behind the nanocrystals on the carbon grid. Further verification of the size of the particles and their crystal structure identification were carried out using X-ray diffraction, recorded on a Siemens D5005 diffractometer using Cu K α radiation. Electron paramagnetic resonance (EPR) spectra of the powder samples of Cu doped ZnO were recorded on an ER 200D X-Band Bruker instrument at 77 K. The powder samples of Cu doped ZnO nanocrystals were dissolved in i-PrOH and the bandgaps were determined from the optical absorption spectra obtained using Perkin Elmer double beam LM-35 spectro-photometer. Pure i-PrOH was used as the reference blank solution for the samples. Fluorescence spectra were obtained using a Perkin Elmer LM-55 spectrofluorophotometer after dissolving the powders in i-PrOH.

UV-Absorption spectra, Photoluminescence and EPR spectra of 2% Cu doped ZnO before and after etching with H₂O₂.

UV-Absorption and its derivative

Photoluminescence

EPR

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UV-absorption data for capped and free standing Cu doped ZnO.

UV-Absorption for different x -values of capped $\text{Zn}_{1-x}\text{Cu}_x\text{O}$ nanocrystals.

UV-Absorption for different x -values of free standing $\text{Zn}_{1-x}\text{Cu}_x\text{O}$ nanocrystals.

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