

Supplementary data

Nucleation and growth of surfactant passivated CdS and HgS NPs: Time dependent Absorption and Luminescence profiles

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Determination of optical band gap

The optical band gap of CdS and HgS NPs has been evaluated from the absorption spectrum using the Tauc relation [1]

$$(\epsilon h\nu) = C(h\nu - E_g)^n \quad (1)$$

where C is a constant, ϵ is molar extinction coefficient, E_g is the average band gap of the material and n depends on the type of transition. For $n = 1/2$, E_g in equation (1) is direct allowed band gap. The average band gap was estimated from the intercept of linear portion of the $(\epsilon h\nu)^2$ vs. $h\nu$ plots on $h\nu$ axis as shown in Figure S1. The band gap values has been found to be higher than the value of bulk CdS (2.42 eV) and HgS (2.0 eV) due to quantum confinement.

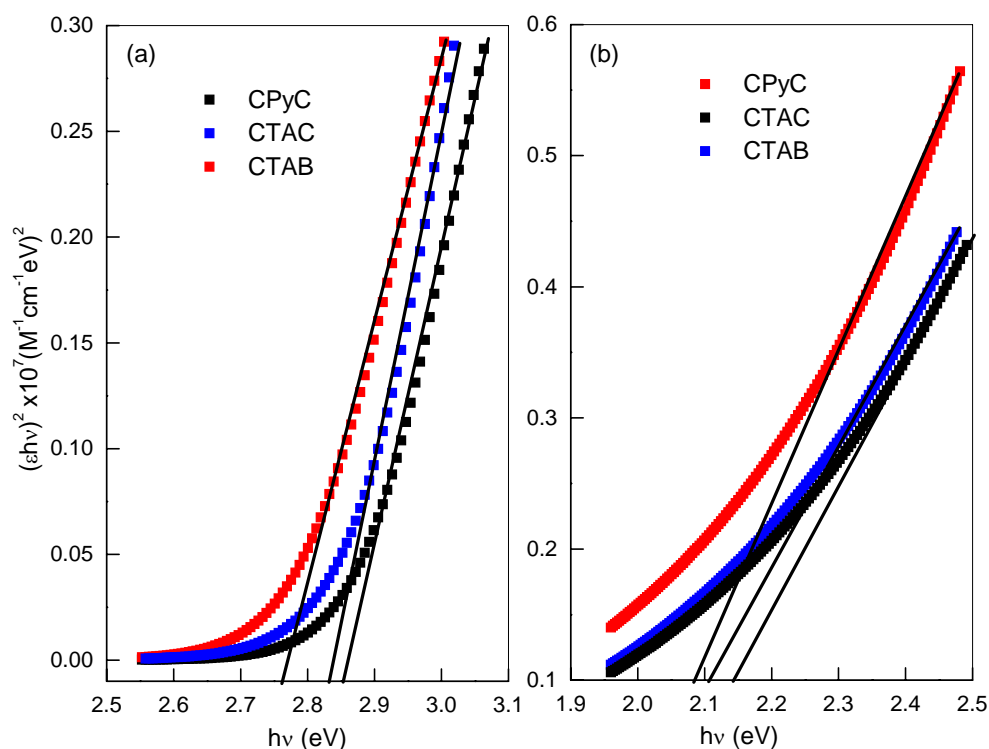


Figure S1. Tauc plots for the determination of optical band gap for (a) CdS NPs and (b) HgS NPs prepared in aqueous micellar solution of three surfactants

Comparative Powder X-ray diffractions of CdS and HgS NPs in three cationic surfactants

The CdS and HgS NPs were separated from the aqueous micellar solutions of CTAB, CTAC and CPyC by evaporating the solvent at 50-55°C. Then, the obtained washed with water and then with ethanol repeatedly to remove excess surfactant and dried. The X-ray diffraction patterns of CdS NPs and HgS NPs separated from the three surfactants are shown in Figures S2 and S3 respectively. The XRD patterns as well as the line broadening in all the three samples seem to be identical with little difference in smoothness due to some incomplete removal of surfactant from the sample.

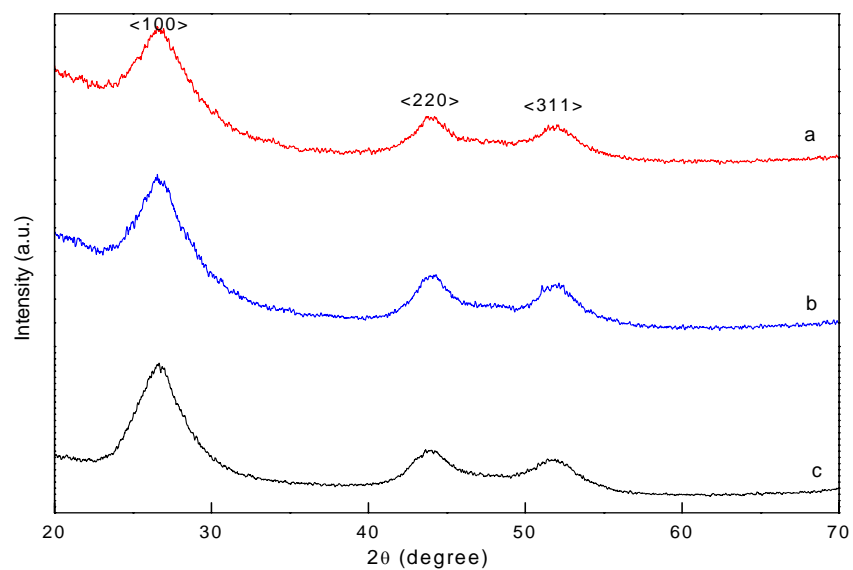


Figure S2. XRD diffraction patterns of CdS NPs separated from aqueous micellar solution of (a) CPyC, (b) CTAC and (c) CTAB.

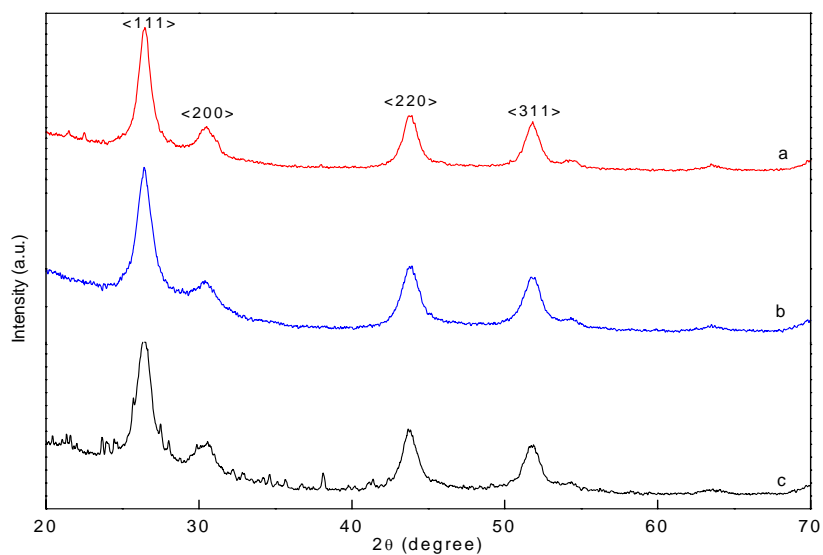


Figure S3. XRD diffraction patterns of HgS NPs separated from aqueous micellar solution of (a) CPyC, (b) CTAC and (c) CTAB.

Time dependent UV-vis absorption spectra of CdS and HgS NPs

Figures S4 and S5 represent red shift in UV-visible spectra of CdS and HgS NPs in aqueous solution of three surfactants, as a function of time, respectively. In these studies, the NPs were produced by rapid mixing of two aqueous micellar solutions, one containing metal cations and other containing S^{2-} ions. The solutions were then immediately transferred in to quartz cuvette for UV-visible spectroscopy. The mixing time was about 30-35 s before taking the spectra. The measurements were then carried out at an interval of 2 minutes.

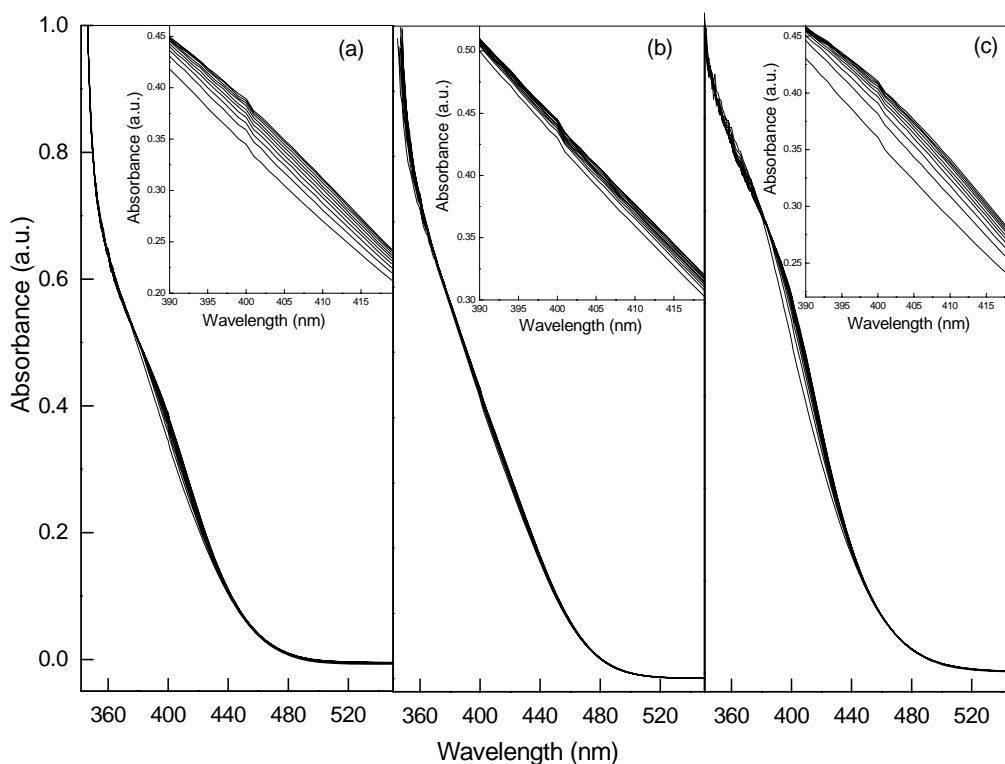


Figure S4. Change in UV-vis absorption spectra with time, of CdS NPs in 3 mM aqueous solution of (a) CTAB, (b) CTAC and (c) CPyC. Magnified views of a portion of absorption spectra undergone prominent shift are shown as inset.

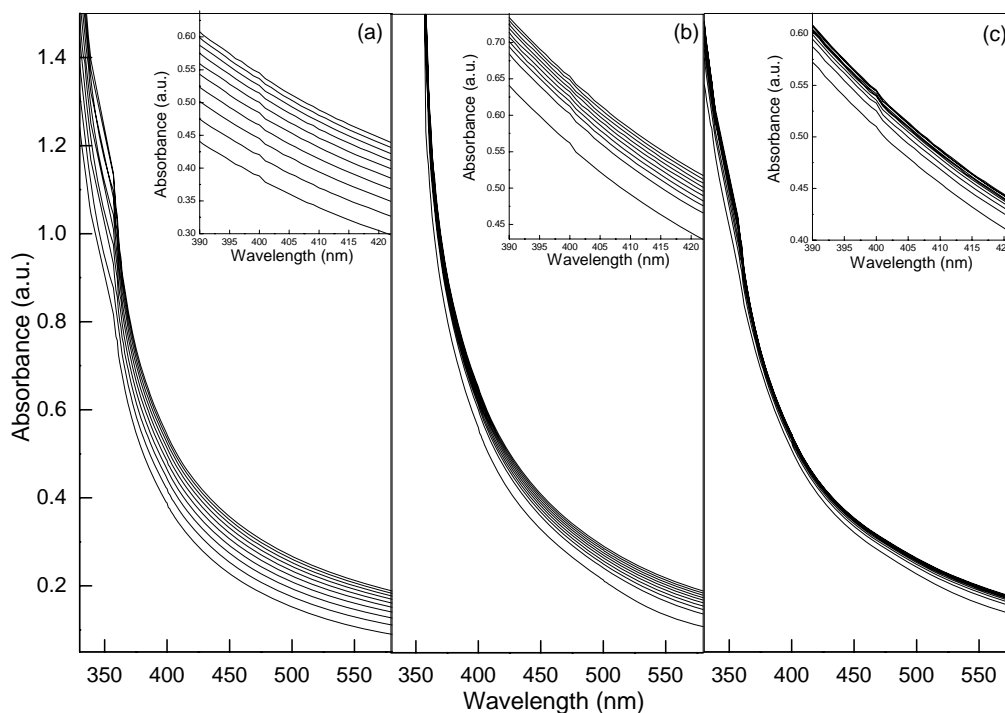


Figure S5. Change in UV-vis absorption spectra with time, of HgS NPs in 3 mM aqueous solution of (a) CTAB, (b) CTAC and (c) CPyC. Magnified views of a portion of absorption spectra undergone prominent shift are shown as inset.

Time dependent PL emission spectra of CdS NPs

Figure S6 Shows PL emission spectra of CdS NPs in aqueous solution of three surfactants recorded at different time intervals during growth process. For these studies, the NPs were produced by mixing of two aqueous micellar solutions, one containing Cd^{2+} and other containing S^{2-} ions. The solutions were then immediately transferred in to quartz cuvette for PL spectroscopy. The mixing time was about 30-35 s before recording the spectra. The measurements were then carried out at an interval of 2 minutes keeping the sample in the spectrophotometer excited at 380 nm.

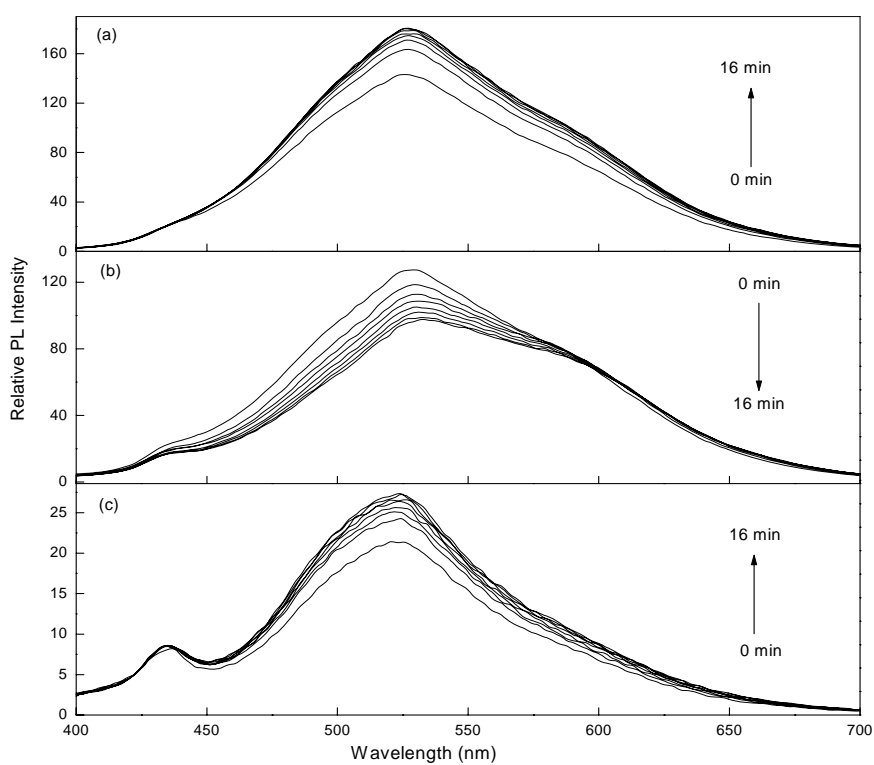


Figure S6. Changes in PL emission spectra of CdS NPs with time, in 3 mM aqueous solution of (a) CTAB, (b) CTAC and (c) CPyC.

Reference:

[1] Tauc J, Menth A 1972 Non Cryst. Solids **569** 8