Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supplemental Information

"*Understanding quantum confinement and ligand removal in solution-based ZnO thin films from highly stable nanocrystal ink* "

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1. Synthesis of ZnO nanocrystals

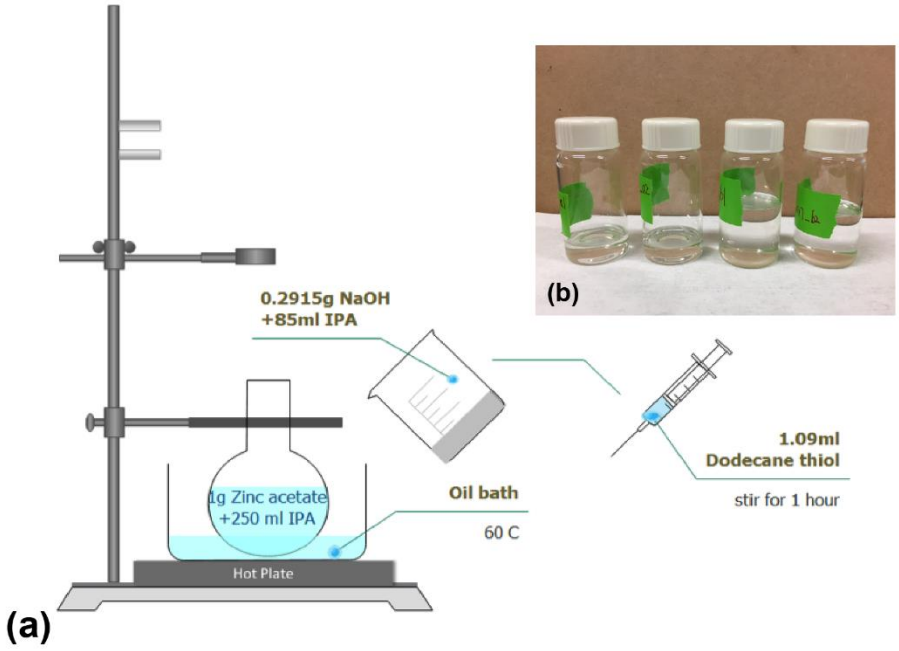

Fig. S1 (a) Schematic of ZnO nanocrystal synthesis (b) ZnO nanocrystal ink of different concentrations

2. Model of particle size from measured absorbance data

In addition to extracting the band gap, the absorption spectrum can also be used to estimate the nanocrystal size. Meulenkamp proposed a method to correlate the particle size with the wavelength at which the absorbance is 50% of the peak value, referred to as $\boldsymbol{\lambda_{1/2}}$. From Figure 2, $\boldsymbol{\lambda_{1/2}}$ = 353 nm for our ZnO nanocrystals. Using Meulenkamp's expression:

$$\boldsymbol{1240/\lambda_{1/2} = 3.301 + 294/D_{uv-vis}^{2} + 1.09/D_{uv-vis}}$$

gave a particle diameter from the absorption spectrum $\boldsymbol{D_{uv-vis}}$ of 39.3 Å. This value is in excellent agreement with the diameter concluded from the TEM picture ($\boldsymbol{D_{TEM}}$).

3. TEM pictures and histogram of ZnO nanocrystal ink after 7 months storage

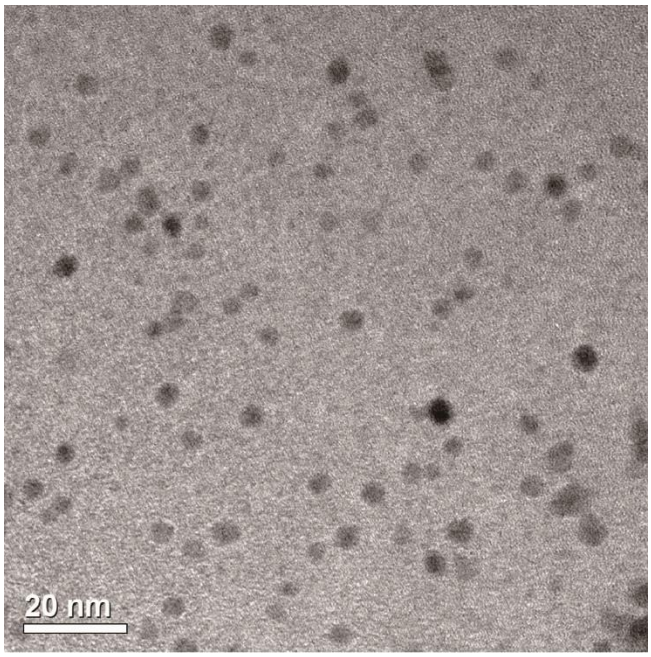

Fig. S2 Transmission electron micrograph (TEM) of dodecanthiol-capped ZnO nanocrystals after 7 months storage

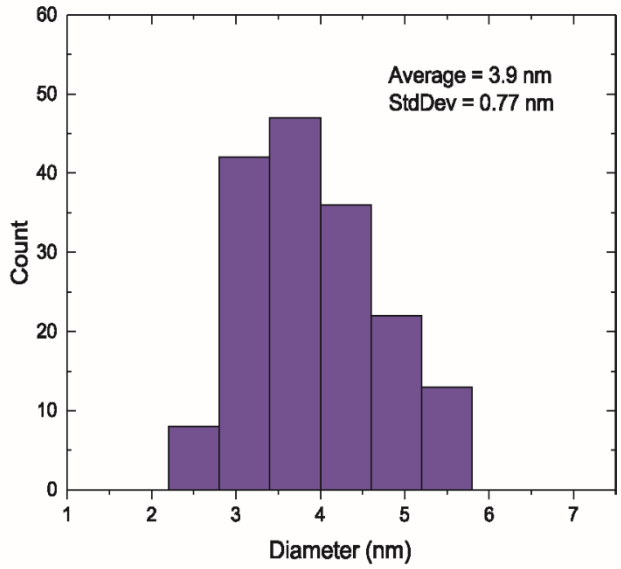

Fig. S3 Histogram of dodecanthiol-capped ZnO nanocrystals after 7 months storage

4. Atomic composition of ZnO nanocrystal thin films from depth profiling with XPS

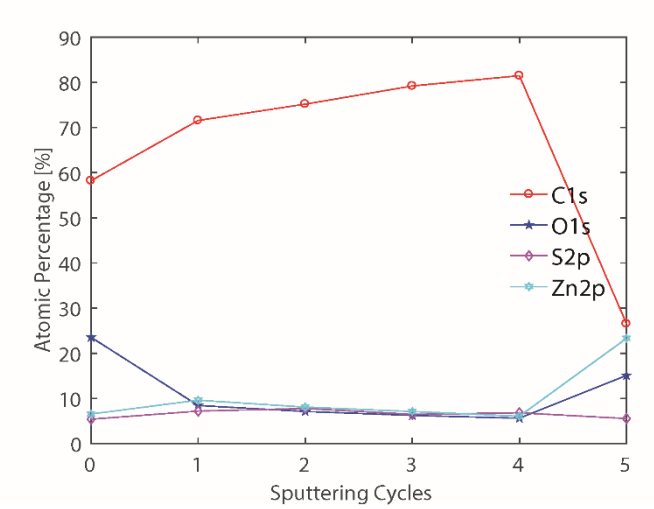

Fig. S4 Atomic composition of as-prepared ZnO nanocrystal thin film

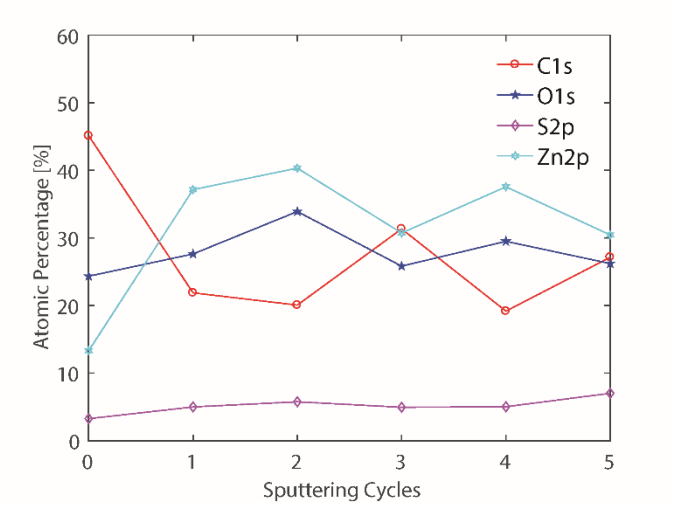

Fig. S5 Atomic composition of ZnO nanocrystal thin film after 150C tube furnace annealing

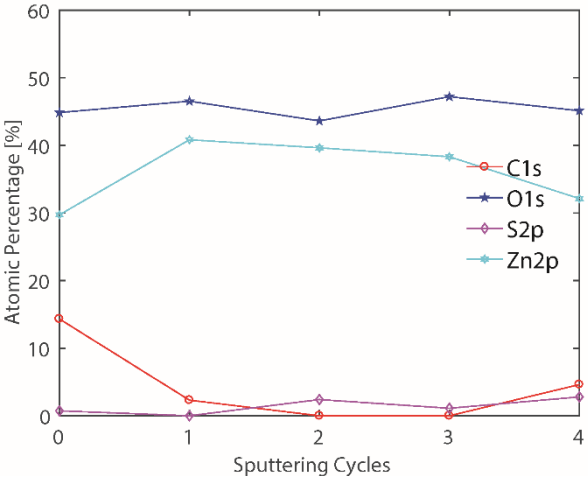

Fig. S6 Atomic composition of ZnO nanocrystal thin film after 300C tube furnace annealing

5. Optical constant and extinction coefficient obtained from VASE measurement

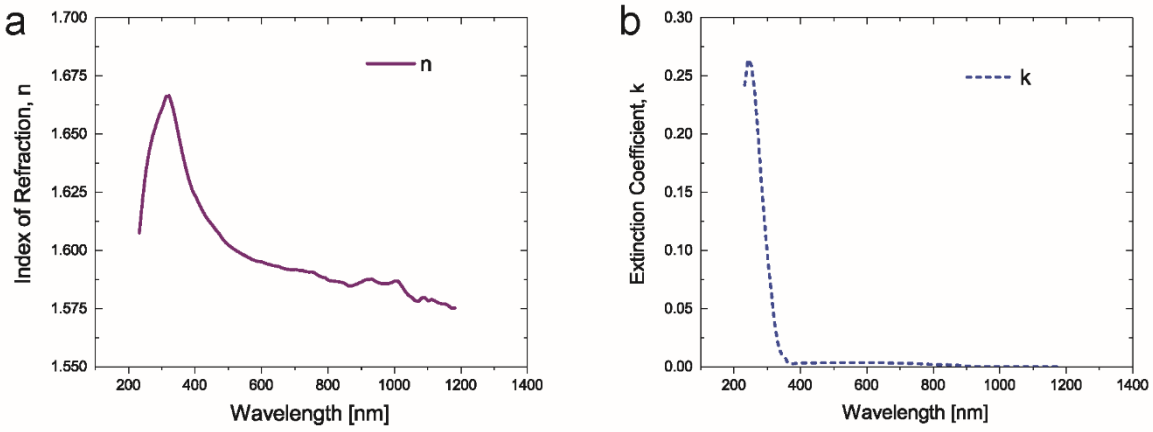

Fig. S7 Optical constants (n and k) calculated from Cauchy model with VASE data of as-prepared ZnO thin film

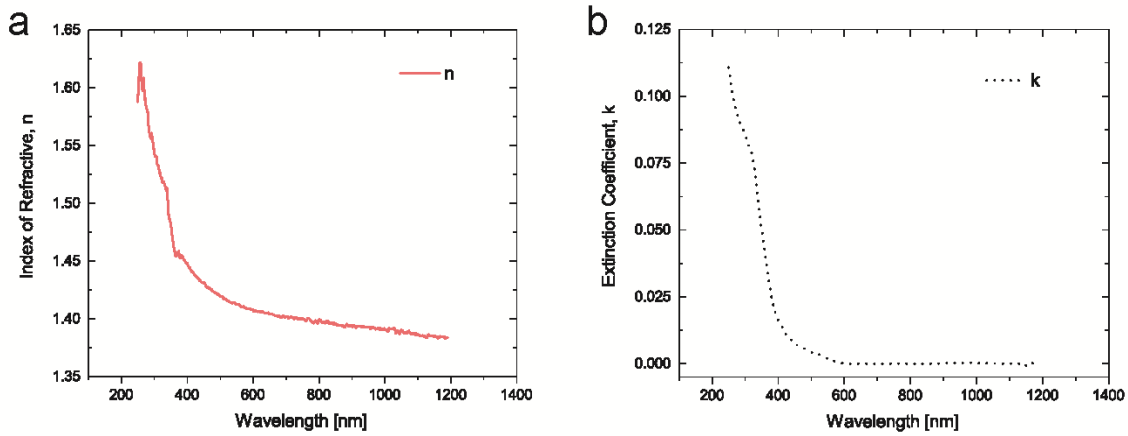

Fig. S8 Optical constants (n and k) calculated from Cauchy model with VASE data of ZnO thin film after 210C annealing

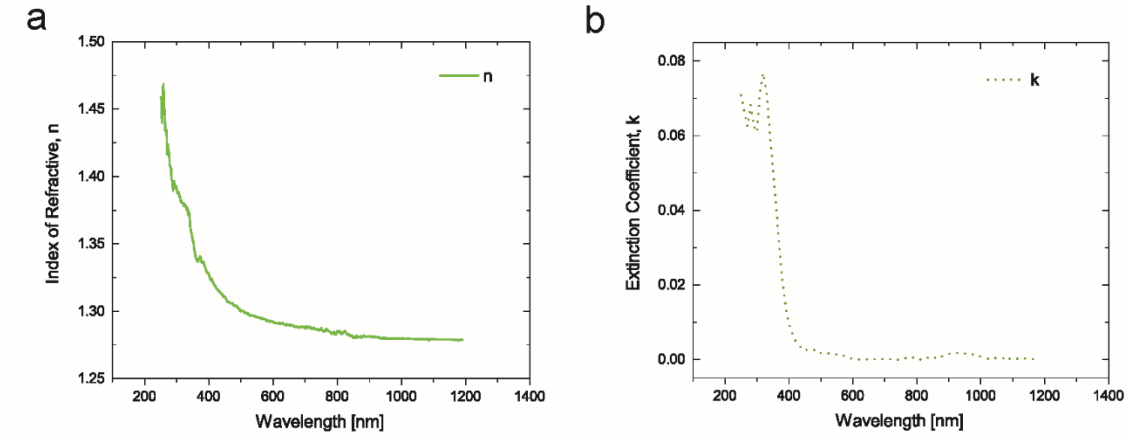

Fig. S9 Optical constants (n and k) calculated from Cauchy model with VASE data of ZnO thin film after 300C annealing