Surface structure, optoelectronic properties and charge transport in ZnO nanocrystal/MDMO-PPV multilayer films

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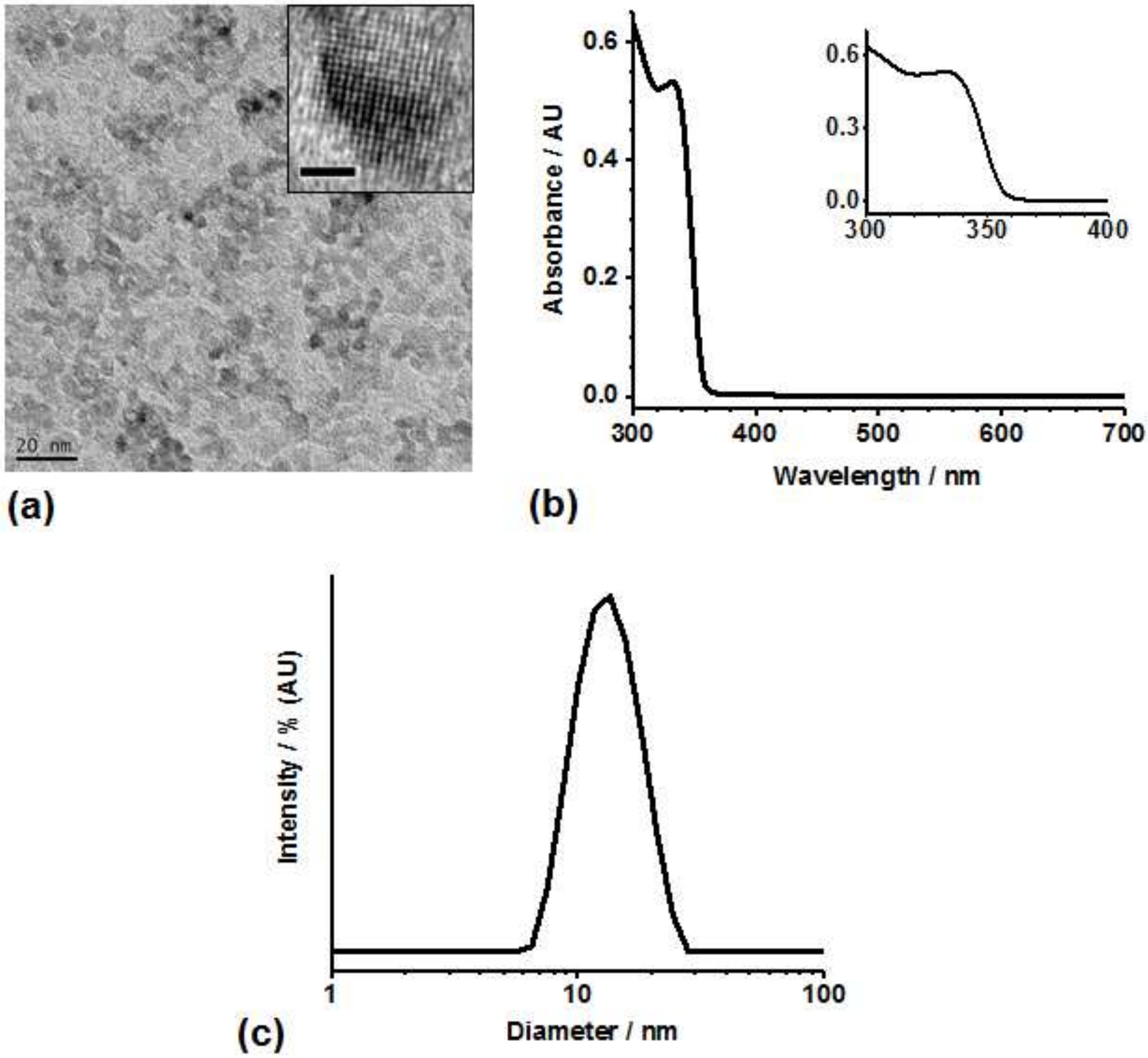

Figure S1. (a) TEM image obtained of deposited ZnO nanocrystals (NCs). The main scale bar is 20 nm. The inset shows a high resolution image of a NC with lattice fringes clearly evident (Inset scale bar: 2 nm). (b) UV-visible spectrum obtained for dispersed ZnO NCs. (c) DLS diameter distribution measured for dispersed ZnO NCs.

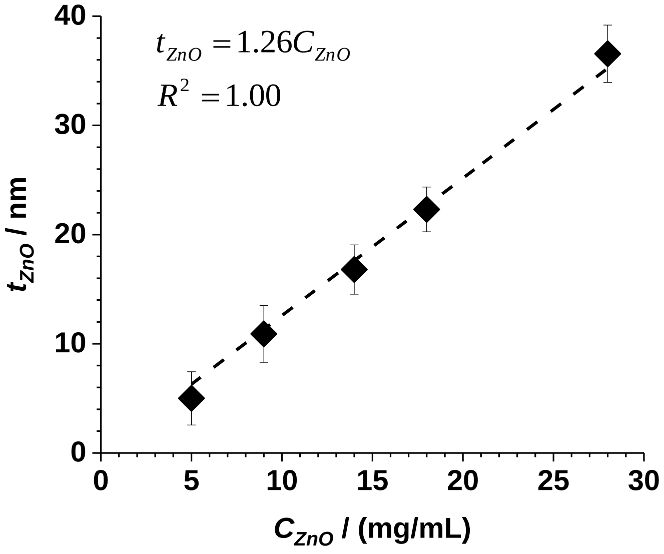

Figure S2. Variation of average ZnO NC layer thickness (t_{ZnO}) with ZnO concentration (C_{ZnO}) used for spin coating. The films were deposited on ITO and one cycle of spin coating was used.

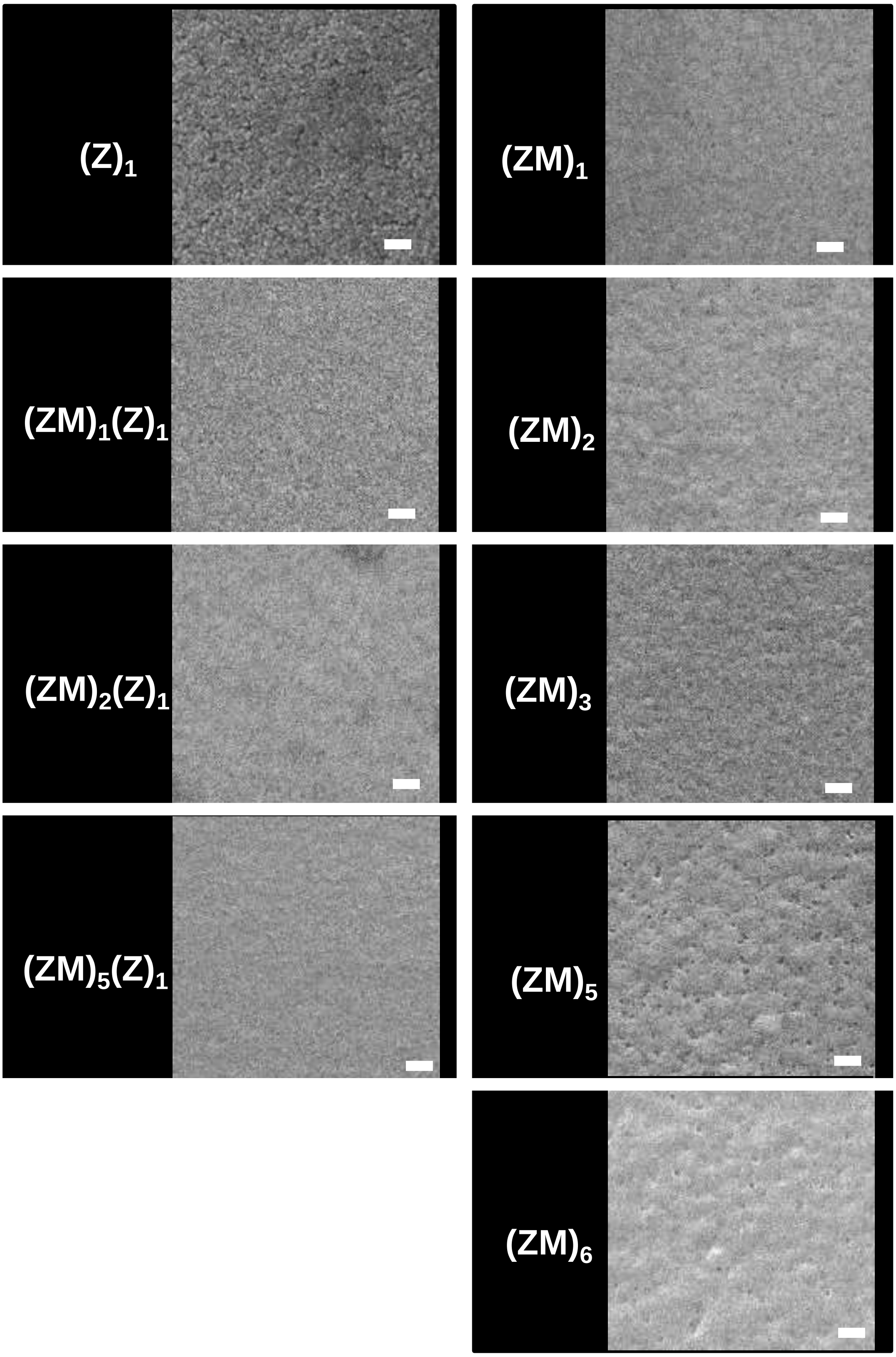

Figure S3. SEM images measured for various multilayer films prepared using C_{ZnO} = 28.0 mg/mL. The top surfaces for the images on the left and right, respectively, were ZnO NCs and MDMO-PPV. Scale bars: 100 nm. SEM images measured for the $(ZM)_3(Z)_1$, $(ZM)_4$ and $(ZM)_4(Z)_1$ films are shown in Fig. 2(a) – (c).

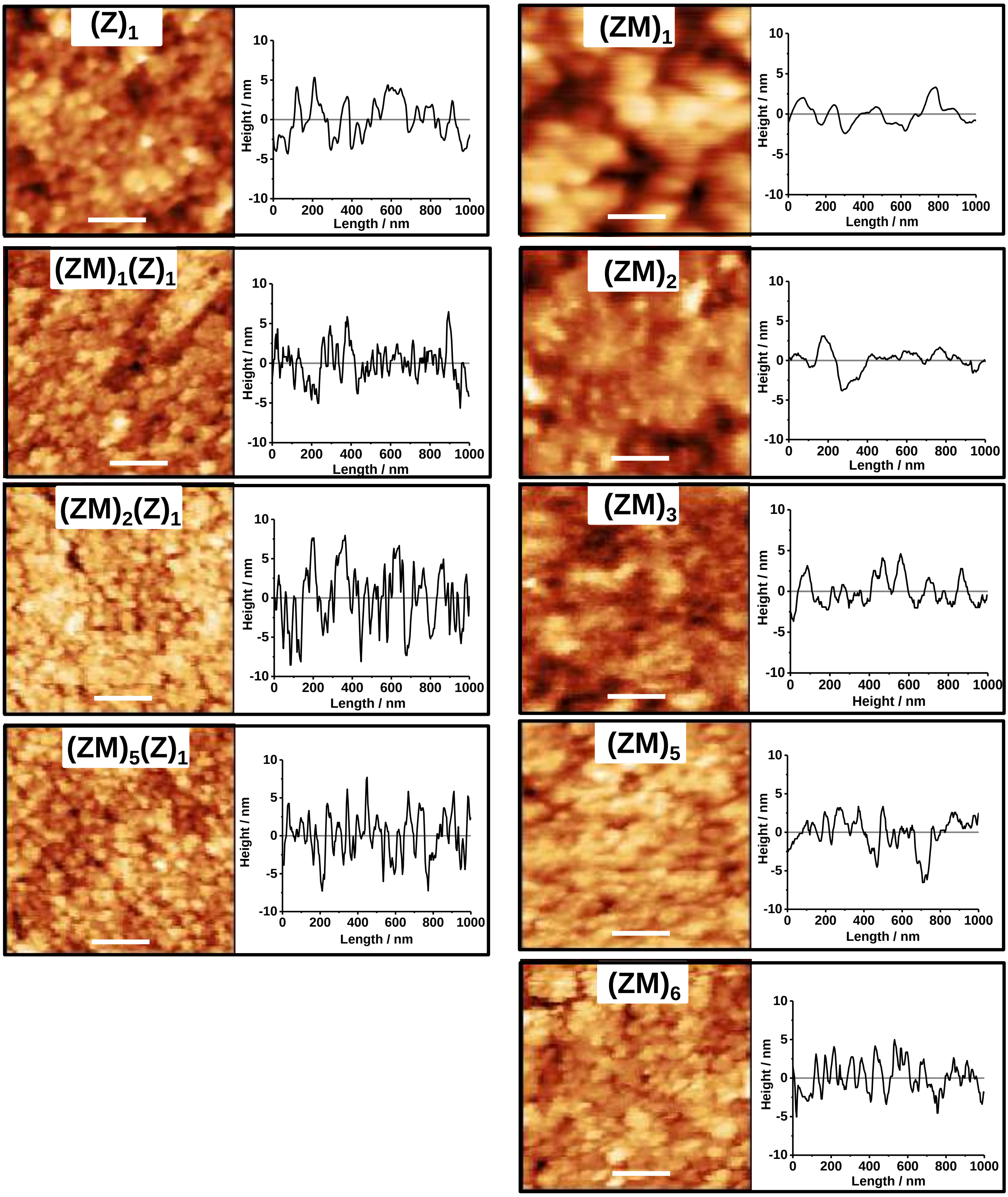

Figure S4. Additional AFM images and line profiles for various multilayer films prepared using C_{ZnO} = 28.0 mg/mL. The images on the left and right show top surfaces that were ZnO NCs and MDMO-PPV, respectively. Scale bars: 100 nm. AFM images and line profiles measured for the $(ZM)_3(Z)_1$, $(ZM)_4$ and $(ZM)_4(Z)_1$ films are shown in Fig. 2(d) – (f).

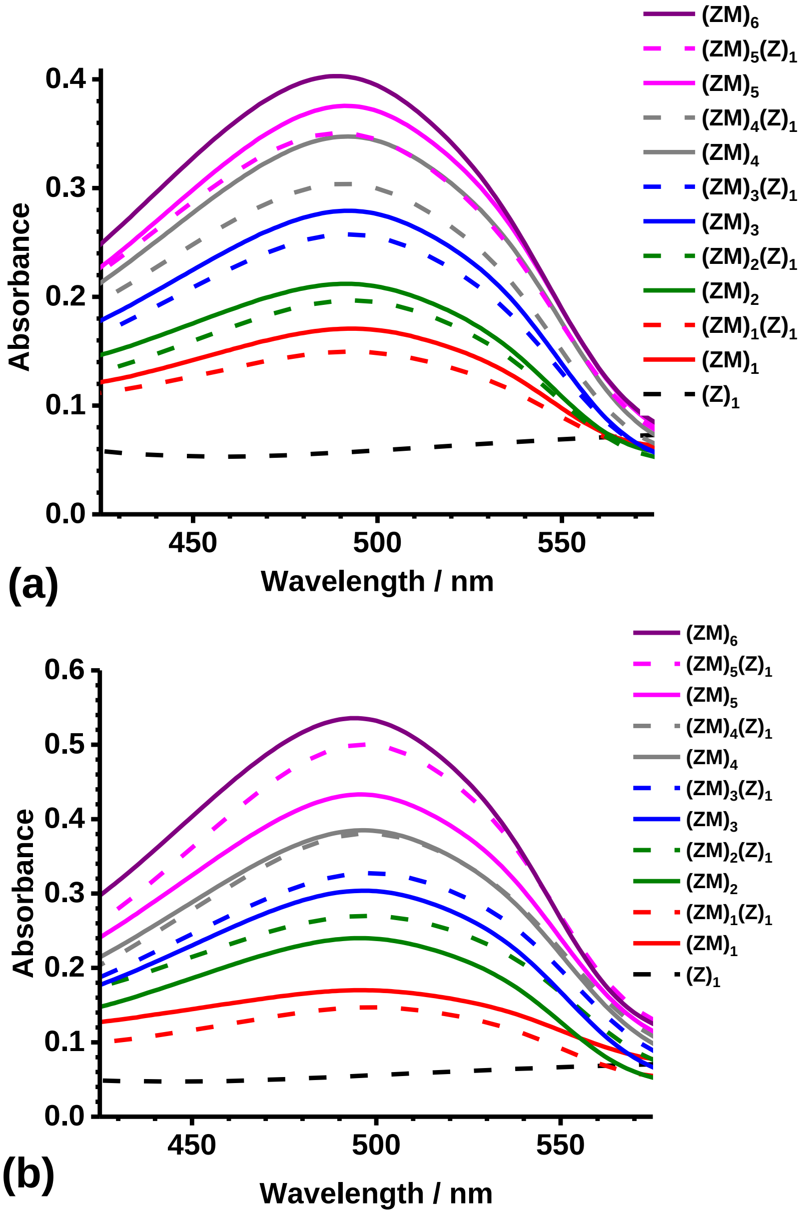

Figure S5. UV-visible spectra measured for ZnO NC/MDMO-PPV multilayer films prepared using C_{ZnO} values of (a) 5.0 and (b) 9.0 mg/mL.

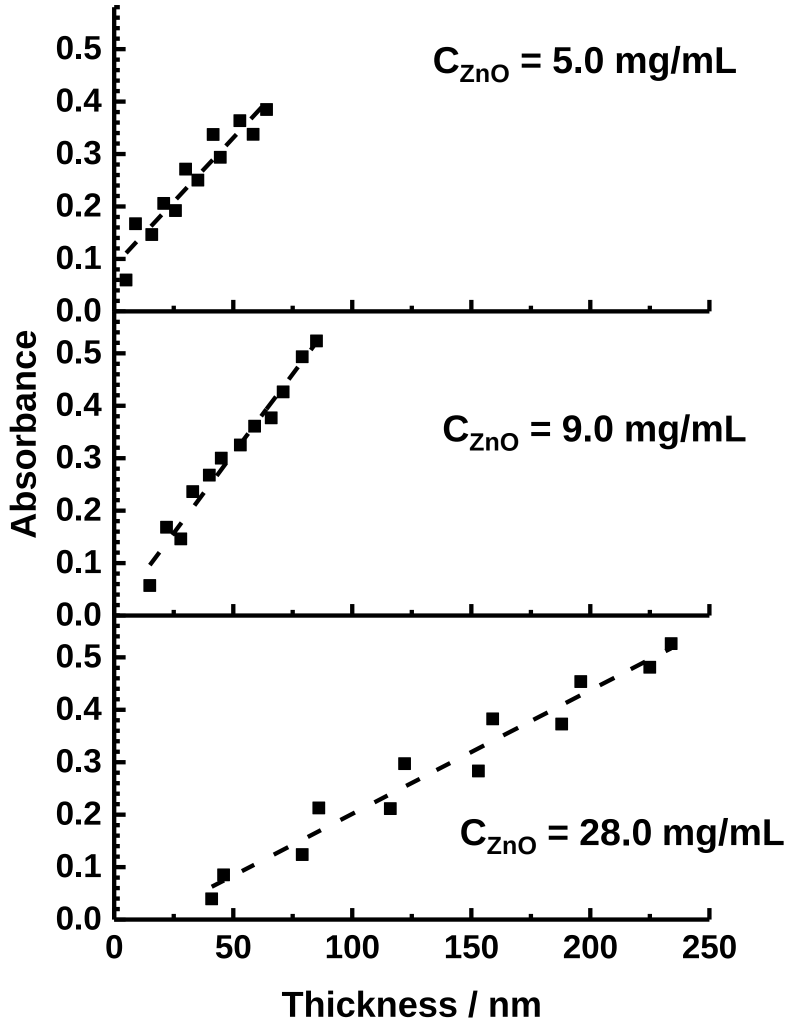

Figure S6. Variation of absorbance measured at 505 nm with thickness for the ZnO NC/MDMO-PPV multilayer films. The gradients were 4.9 x 10^{-3}, 6.1 x 10^{-3} and 2.4 x 10^{-3} nm^{-1} for the films prepared using C_{ZnO} of 5.0, 9.0 and 28.0 mg/mL, respectively.

Calculating the ideal MDMO-PPV volume fraction in multilayer ZnO NC/MDMO-PPV films

The following describes the derivation of an equation that allows the calculation of the ideal volume fraction of MDMO-PPV ($\phi_{MDM(Ideal)}$) in a multilayer ZnO NC/MDMO-PPV film. It is assumed that the area covered by each ZnO NC layer or MDMO-PPV layer (A) are the same. It is also assumed that the ZnO NCs pack perfectly and there was no mass loss during spin coating of an ideal multilayer film. The mass of ZnO NCs (m_{ZnO}) or MDMO-PPV (m_{MDM}) deposited for each layer was

$$m_i = c_i V_{Tot(i)} \qquad \text{(S1)}$$

where c_i and $V_{Tot(i)}$ are the concentrations (mg/mL) and total volumes (mL) of the ZnO NC or MDMO-PPV solutions used to spin coat each layer type. The volume of ZnO NCs (V_{ZnO}) or MDMO-PPV (V_{MDM}) deposited after solvent evaporation is given by

$$V_i = \frac{m_i}{\rho_i} \qquad \text{(S2)}$$

where m_i and ρ_i are the masses and densities, respectively, of the ZnO NCs and MDMO-PPV. Next, the ideal thicknesses of the ZnO NC layer ($t_{ZnO(Ideal)}$) or MDMO-PPV ($t_{MDM(Ideal)}$) layers were calculated using

$$t_{i(Ideal)} = \frac{V_i}{A} \qquad \text{(S3)}$$

It is then straightforward to calculate $\phi_{MDM(Ideal)}$ using the following equation.

$$\phi_{MDM(Ideal)} = \frac{t_{MDM(Ideal)}}{t_{MDM(Ideal)} + t_{ZnO(Ideal)}} \qquad \text{(S4)}$$

Combination of equations (S1) to (S4) enabled the following equation to be obtained.

$$\phi_{MDM(Ideal)} = \frac{1}{1+\left(\frac{c_{ZnO}V_{Tot(ZnO)}\rho_{MDM}}{c_{MDM}V_{Tot(MDM)}\rho_{ZnO}}\right)} \qquad \text{(S5)}$$

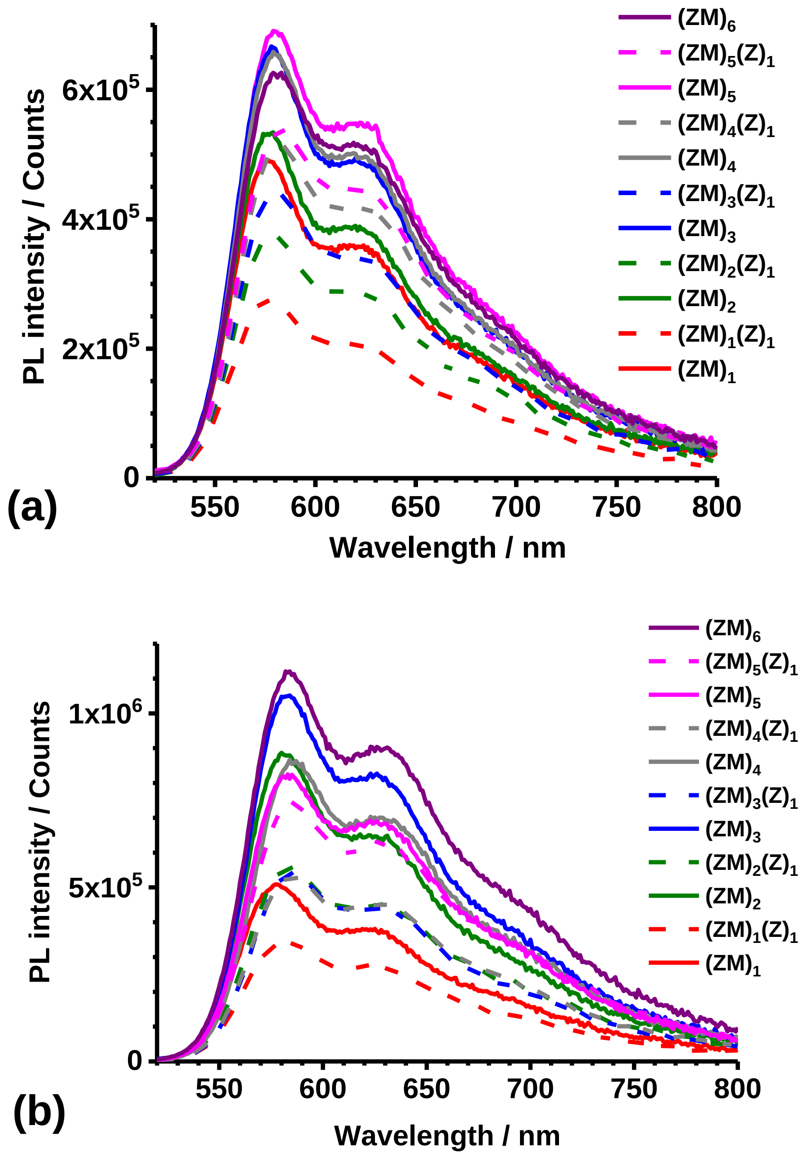

Figure S7. Photoluminescence spectra for ZnO NC/MDMO-PPV multilayer films prepared using C_{ZnO} values of (a) 5.0 and (b) 9.0 mg/mL.

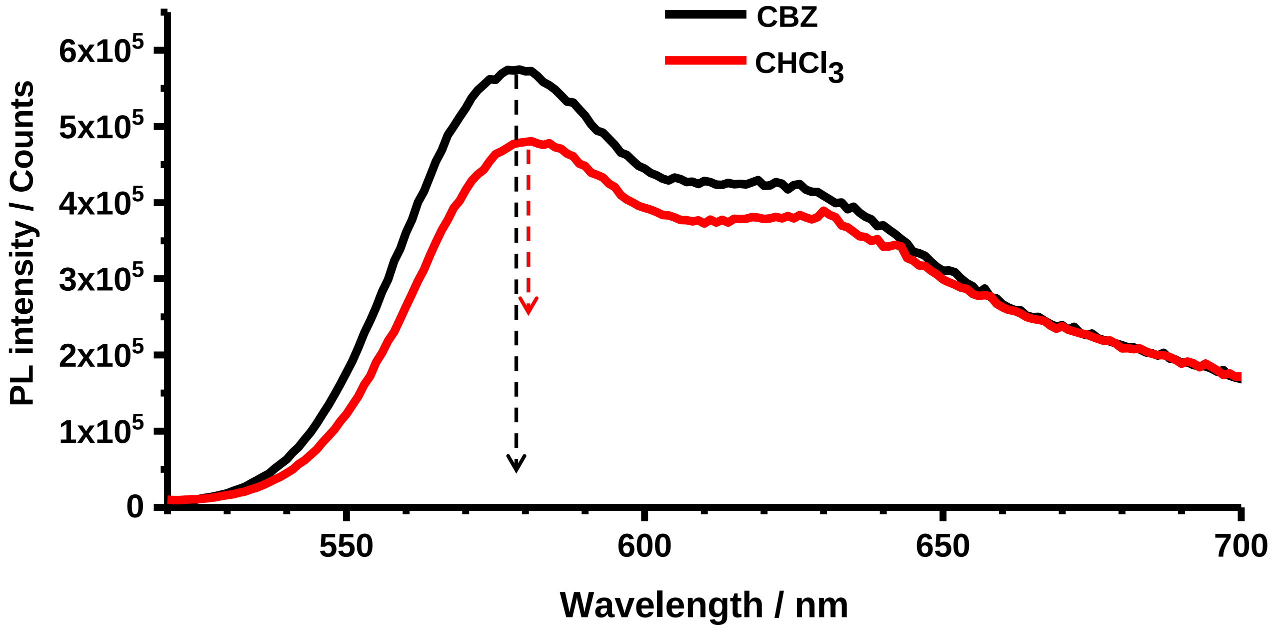

Figure S8. PL spectra for a MDMO-PPV film spin coated from chlorobenzene. A quantity of $CHCl_3$ equivalent to that used during ZnO NC layer coating was then spin coated onto the film and the spectrum re-measured. This treatment caused the wavelength of maximum intensity (λ_{max}) to red shift from 578 to 582 nm.

Table S1. Measured solar cell figures of merit

Device type	C_{ZnO} / (mg/mL)	J_{sc} (mA/cm^{-2})	V_{oc} (mV)	FF (%)	PCE (%)
$(ZM)_6$	5.0	0.21 ± 0.07	666 ± 85	31.1 ± 2.4	0.044 ± 0.014
$(ZM)_6$	9.0	0.25 ± 0.06	705 ± 61	34.7 ± 1.6	0.065 ± 0.019
$(ZM)_6$	14.0	0.22 ± 0.03	796 ± 11	36.4 ± 3.6	0.067 ± 0.010
$(ZM)_6$	18.0	0.20 ± 0.04	709 ± 16	38.1 ± 2.9	0.057 ± 0.010
$(ZM)_3$	14.0	0.19 ± 0.01	422 ± 60	33.8 ± 2.3	0.025 ± 0.005
$(ZM)_1$[a]	28.0	0.20 ± 0.04	686 ± 88	43.0 ± 2.3	0.065 ± 0.019

[a] Bilayer control device.