

## **Interfacial charge transfer dynamics in CdSe/dipole molecules coated quantum dot polymer blends.**

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## **SUPPLEMENTARY INFORMATION**

## 1. CdSe nanocrystal synthesis and ligand exchange.

CdSe quantum dots were synthesized using the wet chemical synthetic method previously described by Nazeeruddin et al. with few modifications <sup>1</sup>. A Se solution was prepared by mixing 0.4g of Se powder, 10 mL of TOP (Trioctylphosphine) and 0.2 mL of anhydrous toluene. 20 g of TOPO (Trioctylphosphine oxide) and 0.25 g of cadmium acetate dihydrate were placed in a round-bottomed flask and heated until 150°C. The solution was purged with argon during the whole reaction. When all the TOPO was dissolved the solution was heated up to 290°C. At this temperature, the Se solution was quickly injected into the reaction vessel through a rubber septum. The heat was removed 15 minutes later and the resulting solution was cooled to room temperature. The CdSe quantum dots were precipitated with a copious amount of methanol and collected by centrifugation and decantation. This purification was repeated three times. The precipitated CdSe quantum dots were recovered by adding Toluene up to a final concentration of 20 mg/mL.

The TOPO capped CdSe quantum dots were then exchanged by several molecules. In the case of the pyridine coated CdSe quantum dots, the TOPO-coated CdSe were dissolved in 40 mL of pyridine and refluxed at 90°C overnight under dark conditions. The substituted benzenethiol-coated CdSe were obtained re-dispersing the TOPO-coated CdSe (1.5 mL) in a mixture of 3.5 g anhydrous toluene and 0.1 mol of each substituted benzenethiol molecule. The solution was refluxed for 24 hours under Ar conditions at 70°C <sup>2</sup>. Finally, the QD were dispersed in Chloroform at 20 mg/mL.

## 2. Morphologic and Spectroscopic measurements.

Atomic Force Microscopy of the samples (AFM) was performed on tapping mode on a Molecular Imaging model Pico SPM II (pico +). Film thickness was measured with an Ambios Technology XP-1 Profilometer.

The UV-Visible spectra were recorded using a Shimadzu UV-1700 spectrophotometer. FTIR Characterization was performed in a NICOLET 5700 FT-IR using a liquids holder with KBr windows. The emission properties were measured under ambient conditions using a Aminco Bowman Series 2 luminiscence spectrometer. Time Correlated Single Photon Counting (TCSPC) experiments were carried out with lifespec.red picosecond fluorescence lifetime spectrophotometer from Edimburg Instruments© equipped with lasers as excitation sources. The instrument response was always shorter than 300 ps measured at full width half maximun (FWHM). Laser Transient Absorption Spectroscopy (L-TAS) were recorded using a home-built system as reported before <sup>3</sup>. The samples were measured with a probe wavelength of 980 nm and an excitation soured of 470nm. Laser intensity pulse was  $86.7 \mu\text{J}/\text{cm}^2$ , repetition rate 1 Hz.

### 3. Photovoltaic device preparation and characterization.

Pre-cleaned ITO (Indium doped tin oxide) substrates were used as anode. A thin layer (30nm) of poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) was deposited by spin coating. The PEDOT:PSS layers were annealed at 100°C in air conditions. Over the PEDOT:PSS layer, the P3HT: CdSe blends were spined, obtaining films of 150 nm, and annealed at 150°C for 30 minutes. Finally, thermal evaporation of 100 nm Al was done at  $10^{-6}$  mbar. The final area of he devices was of  $9 \text{ mm}^2$ .

The I-V characteristics of the devices were carried out automatically with a Keithley model 2600 digital source meter using Labview software.

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- (3) E. Palomares, M. V. M.-D., S.A. Haque, T. Torres, J.R. Durrant. *Chem. Commun.* **2004**, 2112.