Supplementary Material (ESI) for Journal of Materials Chemistry

Supporting Information

The effects of CdSe incorporation into bulk heterojunction solar cells

Jilian Nei de Freitas, Isabel R. Grova, Leni C. Akcelrud, Elif Arici, Niyazi Serdar Sariciftci and Ana Flávia Nogueira[*]

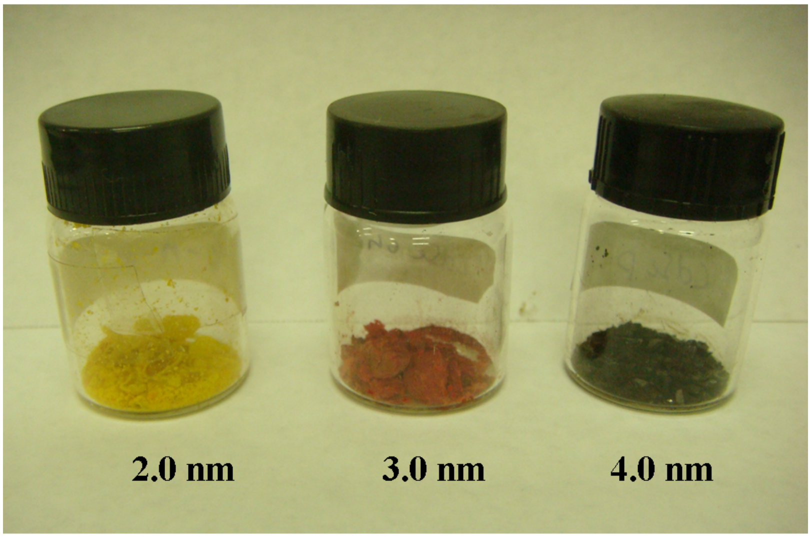

Fig. S1 CdSe nanoparticle powders with different preferential diameters.

Table S1 Diameter of the CdSe nanoparticles synthesized under different conditions (time and temperature). D_{TEM} are the diameters measured from the HRTEM images (30 counts) and D_{abs} is the preferential diameter size estimated from the absorption spectra, using the equation proposed by Yu *et al.*[1].

Synthesis	D_{TEM} (nm)	D_{abs} (nm)
3 min / 260 °C	1.5 – 3.0	2.2
6 h / 260 °C	2.6 – 4.8	3.0
2 h / 340 °C	3.2 – 9.0	4.2

[*] Fax: +55 19 35213023; Tel: +55 19 35213029
* Corresponding author: anaflavia@iqm.unicamp.br

Thin film cyclic voltammetry was employed to estimate the position of HOMO and LUMO of the CdSe nanoparticles. For inorganic nanoparticles, the HOMO values can be estimated from the onset oxidation potentials measured in the voltammograms and the LUMO values can be estimated from the onset reduction potentials. The band gap can be estimated from the absorption spectra, using Tauc's equation[2] (E_g^{opt}) or by the differences in HOMO and LUMO values measured with voltammetry (E_g^{CV}). These methods are well-accepted to estimate the energy levels of inorganic nanoparticles[3-6]. Table S2 presents the values estimated using these methods. The values reported here are similar to those reported in other works, for CdSe nanoparticles with the same sizes[7].

Table S2 HOMO, LUMO and bandgap energy estimated for the CdSe nanoparticles with different sizes.

CdSe preferential size (nm)	**HOMO (eV)**	**LUMO (eV)**	**E_g^{opt} (eV)**	**E_g^{VC} (eV)**
2.0	-5.8	-3.1	2.7	2.6
3.0	- 5.6	- 3.4	2.2	2.3
4.0	-5.5	-3.6	1.9	2.1

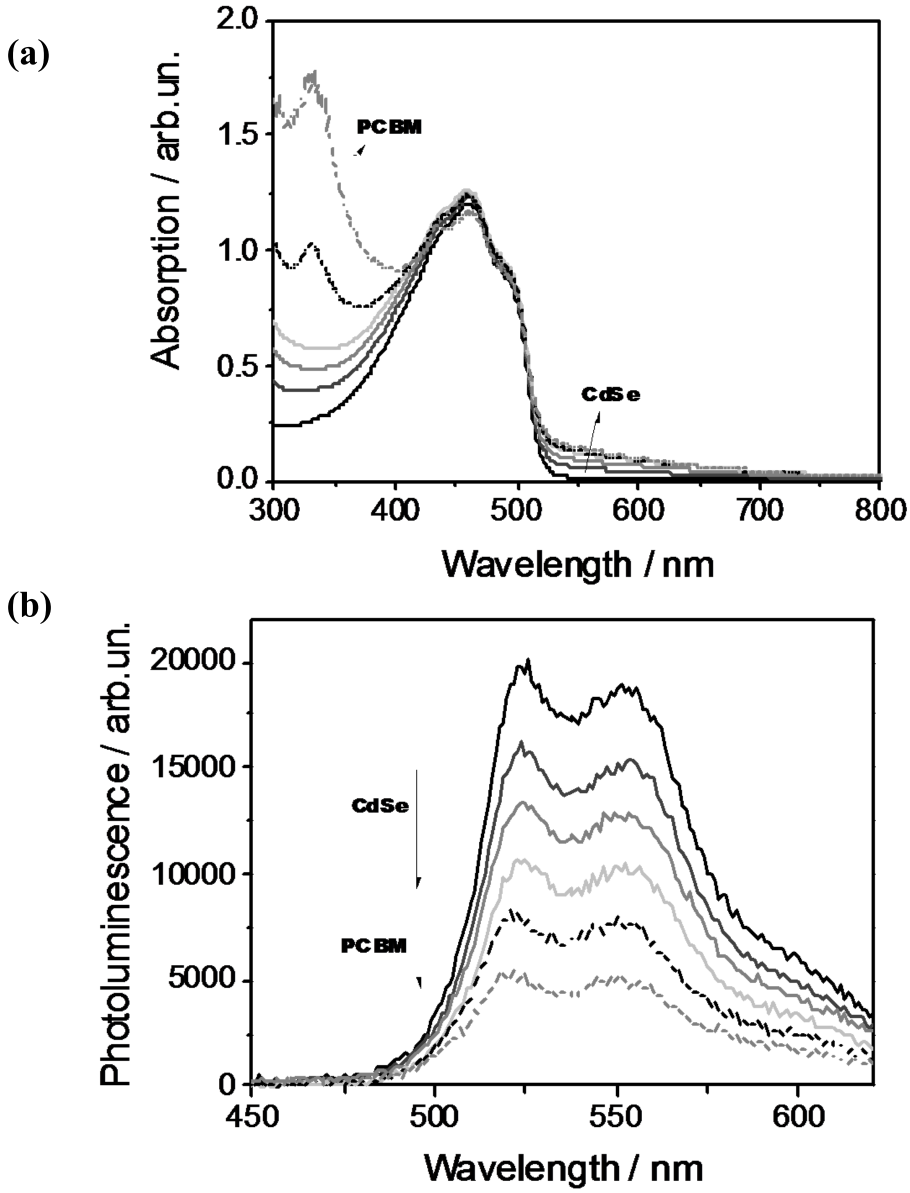

Fig. S2 Absorption (a) and photoluminescence (b) spectra for a solution of PFT in toluene. The quenching of emission is observed even after addition of very small CdSe contents (solid lines). The quenching is further observed after addition of small concentrations of PCBM (dotted lines). This can be considered as a first indication of the existence of charge transfer between the polymer and CdSe nanoparticles. Excitation wavelength = 370 nm.

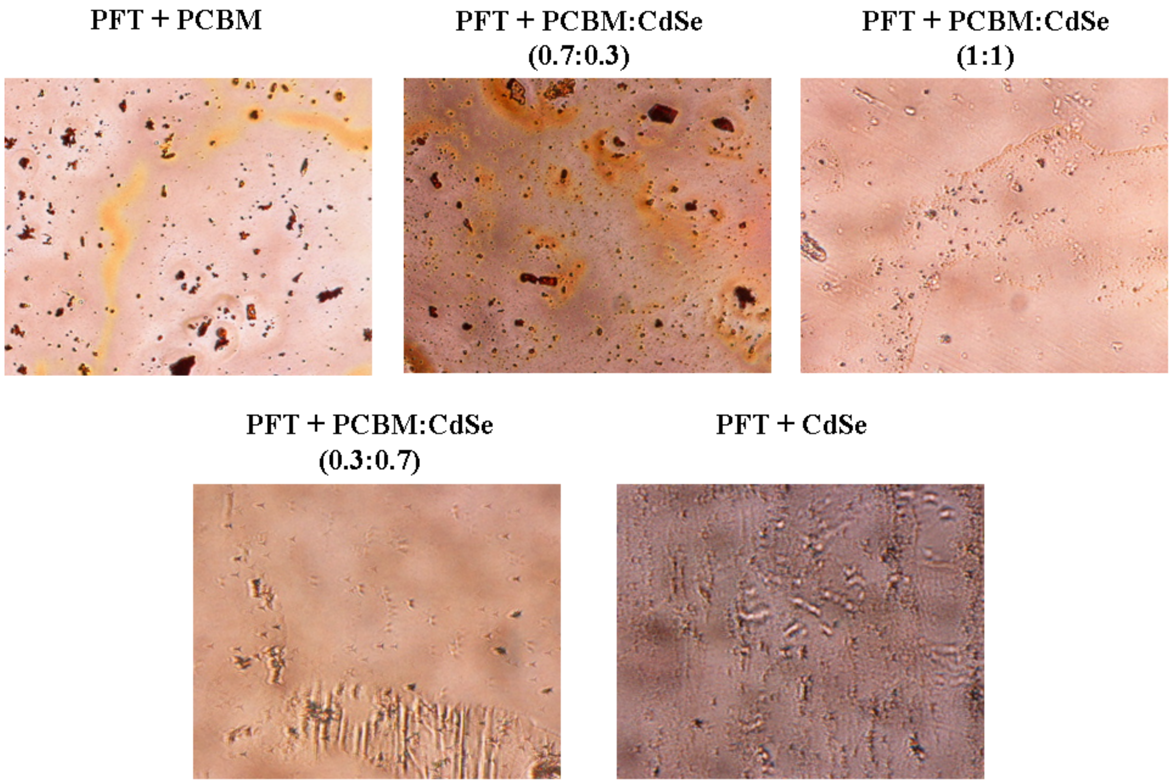

Fig. S3 Optical microscopy images for films of PFT with PCBM and/or CdSe (4.0 nm) with different concentrations, deposited onto PEDOT:PSS covered ITO-glass substrates. The magnification is 40000 times.

Figs. S4 and S5 show J-V curves of solar cells assembled with different active layer compositions. All these devices were assembled under the same conditions: all the assembly and measurements procedures were carried out in air, and the J-V curves were obtained under illumination of 50 mW cm^{-2}.

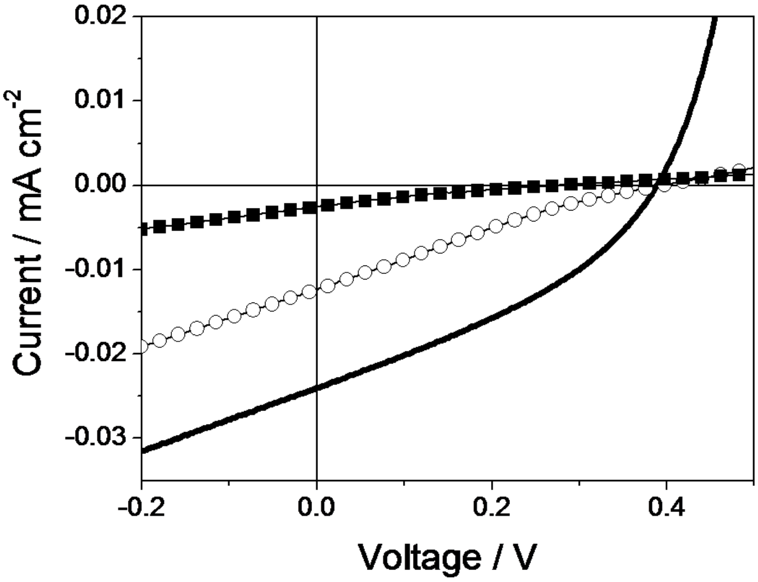

Fig. S4 J-V curves obtained for solar cells based on (—) PFT + PCBM:CdSe (1:1 wt% ratio, corresponding to 40 wt% of CdSe) and the curves obtained for mixtures of PFT + PCBM + TOPO (using the free surfactant as additive), assembled in the same conditions. The concentrations of TOPO were varied between (-○-) 5 and (-■-) 30 wt%. When the TOPO-capped CdSe nanoparticles are substituted for free TOPO, the devices show ohmic behaviors, indicating that the surfactant in the free form acts as an insulator inside the active layer of the device. Therefore, TOPO may not be considered as the responsible for the improvements in the photovoltaic performance of PFT/PCBM/CdSe systems.

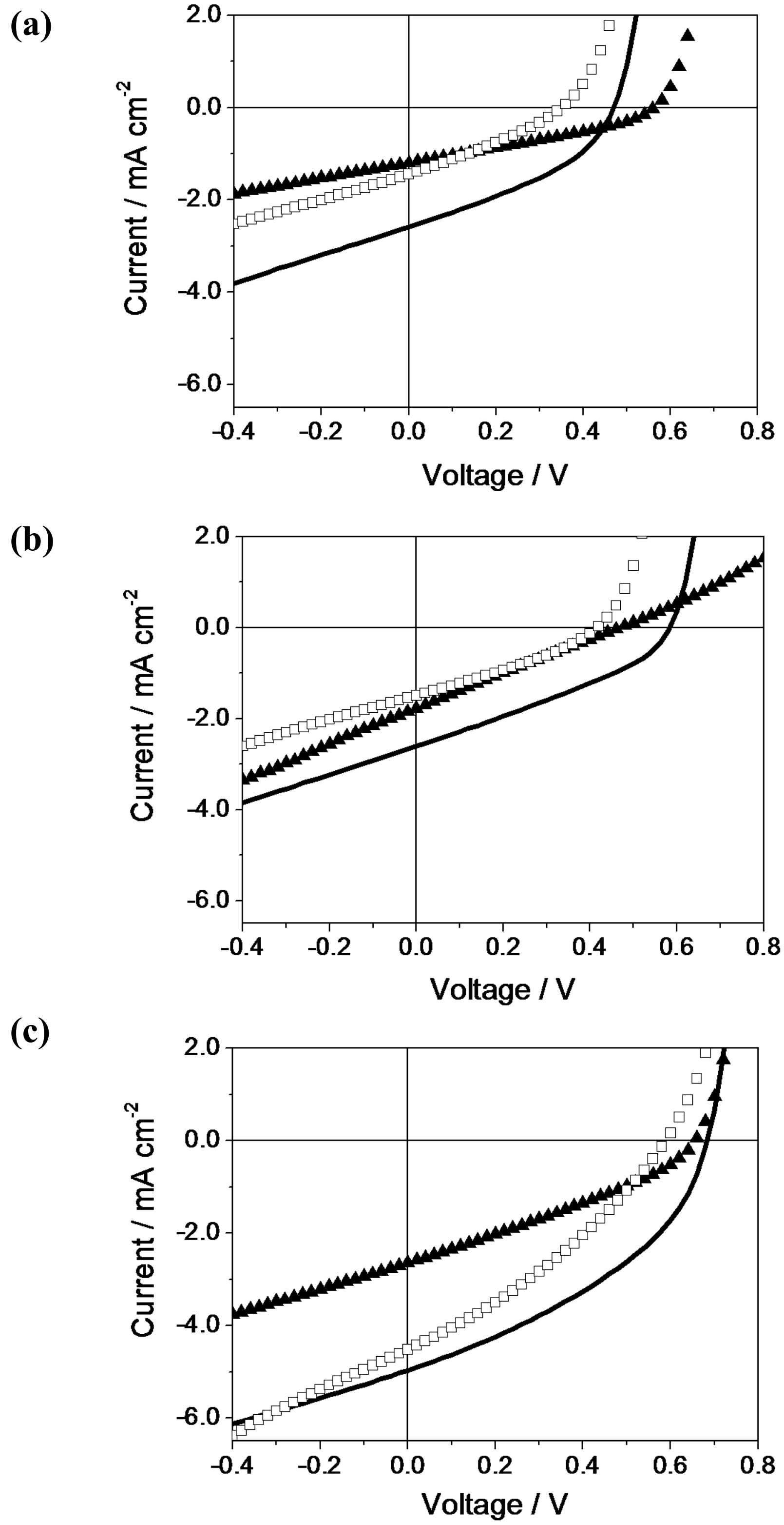

Fig. S5 J-V curves of solar cells assembled with the ternary mixture PFT + PCBM + CdSe, with different material concentrations: (-□-) 0.7:0.3, (▬) 1:1 or (-▲-) 0.3:0.7 wt% PCBM:CdSe ratios, using CdSe nanoparticles with different sizes (a) 2.0 nm, (b) 3.0 nm and (c) 4.0 nm. In all cases, the best performance is obtained for devices assembled with 1:1 PCBM:CdSe ratio.

References

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