



Hybrid solar cells with improved efficiency by ligand exchange with monothiols

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Among the efforts to improve the performance of hybrid solar cells (HSCs), surface engineering of inorganic NCs has been considered as a crucial factor that greatly influences the performance of HSCs.¹ Especially, the nonconductive surfactants on the surface of as-synthesized NCs have disastrous effects on carrier transport in the devices. If the nonconductive surfactants are replaced by short-chain ligands, such as benzene-1,3-dithiol (BDT)² and 1,2-ethanedithiol (EDT)³, the performance of the HSCs will greatly improved.

In this work, we first demonstrated high-performance P3HT:CdSe QDs HSCs fabricated through post-deposition ligand exchange by n-butanethiol (*n*BT), showing PCE as high as 3.09%. We also studied the physical and chemical mechanism for the improvement and demonstrated that the performance of HSCs was highly dependent on the length of ligands tied to the surface of NCs.⁴

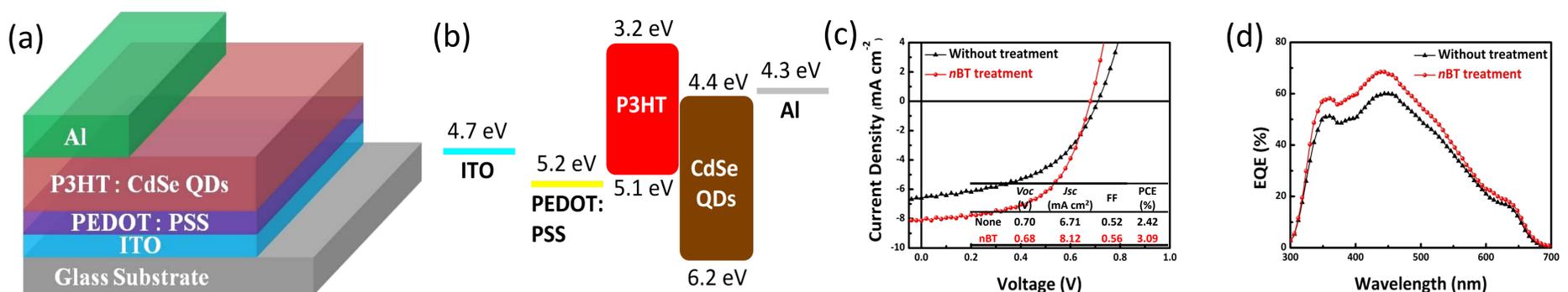


Fig. 1 (a) Schematic of HSCs architecture based on P3HT:CdSe blend; (b) energy level diagram of the corresponding device; (c) *J*-*V* characteristics under simulated 1 sun AM 1.5 solar illumination; (d) EQE for HSCs before and after post-deposition ligand exchange by *n*BT.

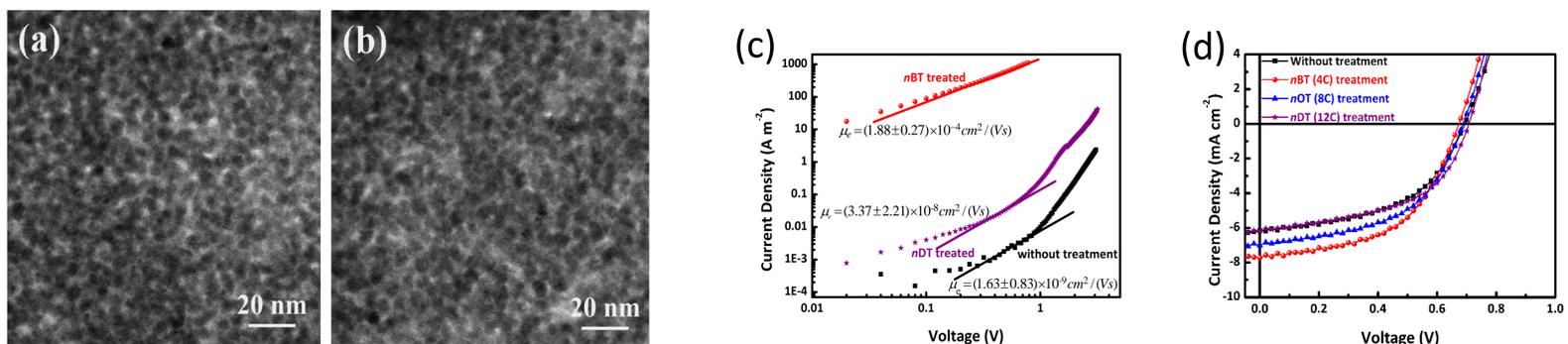


Fig. 2 TEM images of blend films before (a) and after (b) ligand exchange by *n*BT, no obvious changes in phase separation are observed in the film after *n*BT treatment. (c) *J*-*V* characteristics of electron-only devices with a structure of Al/P3HT:CdSe/Al. Electron mobility will be enhanced greatly by *n*BT treatment and enhanced slightly by *n*DT with a longer alkyl chain. (d) *J*-*V* characteristics of hybrid devices treated by monothiols with different chain lengths. The performance of hybrid P3HT:CdSe QDs solar cells was highly dependent on the length of ligands on the surface of CdSe QDs. The CdSe QDs were ~ 6.4 nm in size.

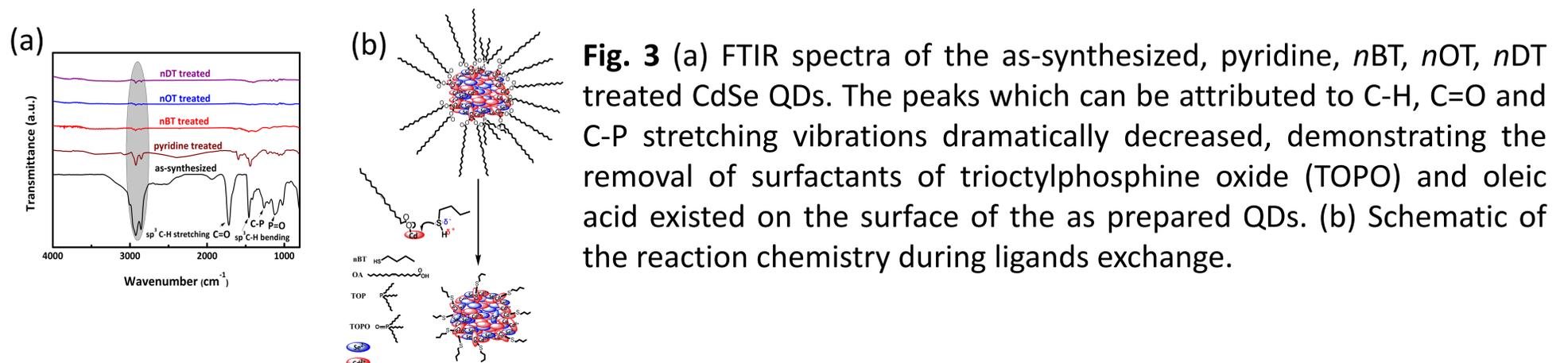


Fig. 3 (a) FTIR spectra of the as-synthesized, pyridine, *n*BT, *n*OT, *n*DT treated CdSe QDs. The peaks which can be attributed to C-H, C=O and C-P stretching vibrations dramatically decreased, demonstrating the removal of surfactants of trioctylphosphine oxide (TOPO) and oleic acid existed on the surface of the as prepared QDs. (b) Schematic of the reaction chemistry during ligands exchange.

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