Electron Tomography of PbS-PTB1 Morphology as a Function of Ligand Exchange

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Abstract

Solution processable organic photovoltaic devices are appealing because of their high potential performance to cost ratio. Traditional all-organic PV devices utilize a conjugated polymer mixed with fullerene molecules as an absorber layer. Recently hybrid organic-inorganic devices using lead sulfide quantum dots instead of fullerenes have been investigated. PbS nanoparticles are advantageous due to their low and tunable band gap, wide range of absorption into the infra-red, thermal stability, reduced recombination rate and longer carrier lifetimes. The morphology of these devices is critical to their performance. Coarse measurements such as average domain size don't provide the most relevant information to device performance, namely the distance distribution between donor and acceptor regions in the volume. To obtain more detailed morphological information, a 3D reconstruction of the film is created via high angle annular dark field electron tomography using a scanning transmission electron microscope. The effect of different ligand exchange procedures on the film morphology is investigated.

PbS/PTB1 Device Performance

2.8% Overall efficiency for non-optimized devices

Size dependent PbS band gap affects charge transfer

How can the device be optimized for charge separation and transport?

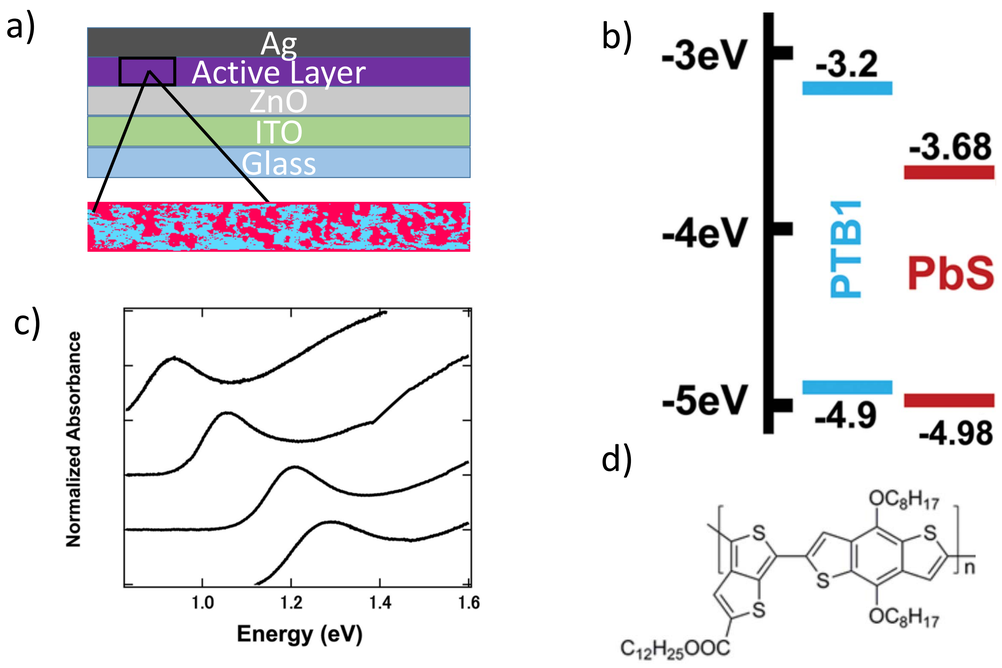

Figure 1. a) Device schematic with inset of cross-sectional active layer morphology. b) Energy levels of PTB1 and PbS particles. C) Absorption spectra for different sizes of PbS particles. d) Chemical structure of poly((4,8-bis(octyloxy)benzo(1,2-b:4,5- b) dithiophene-2,6-diyl)(2-((dodecyloxy)carbonyl)thieno(3,4- b)thiophenediyl)) (PTB1) [1]

Device Fabrication

Spin cast from solution

Ligand exchange necessary for charge transport between particles

How do ligand exchange and processing conditions affect device morphology and performance?

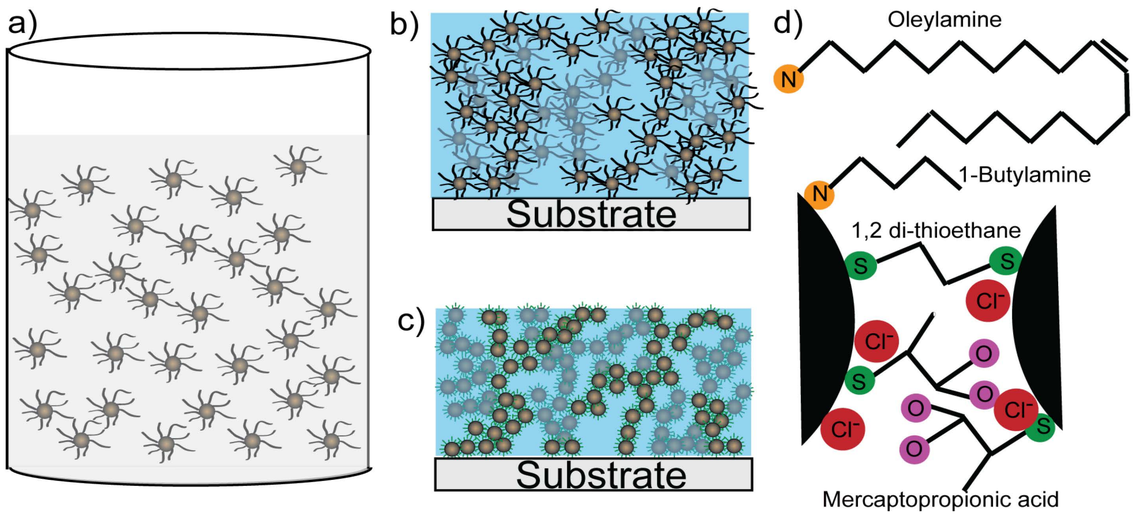

Figure 2. a) Quantum dots synthesized with long chain ligands. b) PbS/polymer solution cast onto substrate. c) Ligand exchange performed using orthogonal solvent with smaller, more strongly binding ligands. D) Example of large capping ligand (oleylamine), intermediate ligand (butylamine), and short ligands (mercaptopropionic acid and dithioethane).

Measuring 3D Nano-scale Morphology

High angle annular dark field scanning transmission electron microscopy

Series of projection images taken at different angles used to reconstruct a "best fit" volume

PbS/PTB1 treated as two-phase system, no mixed phase

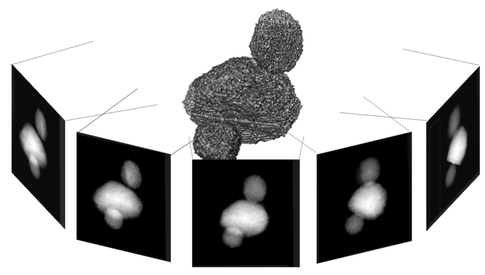

Figure 3. Example of a projection tilt series. Multiple angles are necessary since a single projection could result from a nearly infinite number of different objects; a unique 3D solution can be found only with a wide range of angles.

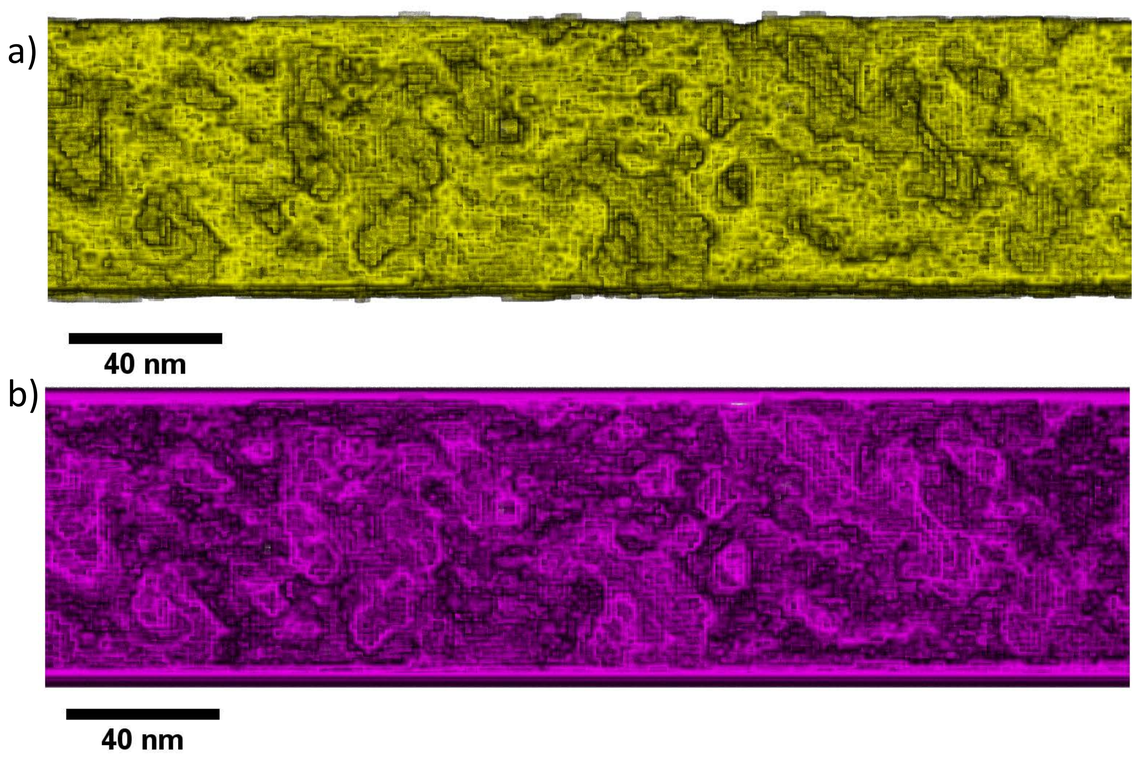

Figure 4. 3D reconstruction of PbS/PTB1 film after two ligand exchanges: oleylamine to butylamine and butylamine to MPA.
a) PbS domains in yellow and b) PTB1 domains in purple

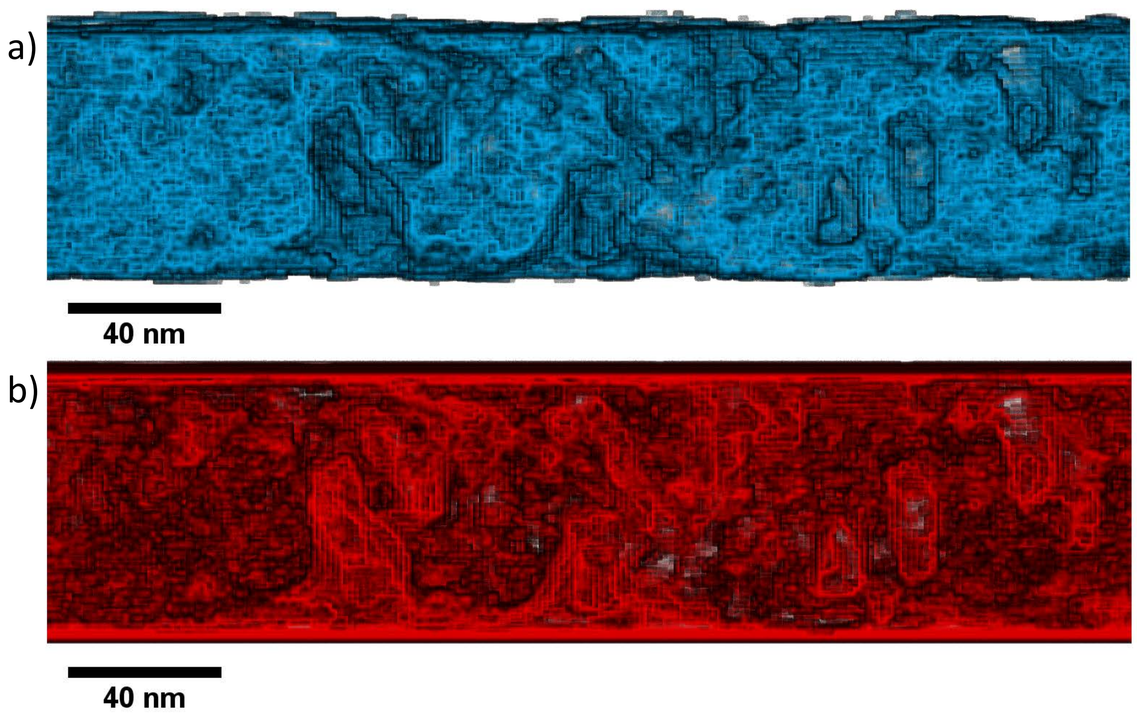

Figure 5. 3D reconstruction of PbS/PTB1 film after a single ligand exchange: oleylamine to MPA.
a) PbS domains in blue and b) PTB1 domains in red

Acknowledgements

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References

1. Nagaoka, Hirokazu, et al. "Size-dependent charge transfer yields in conjugated polymer/quantum dot blends." *The Journal of Physical Chemistry C* 118.11 (2014): 5710-5715.