Integration of Molecular Imaging Techniques to Probe the Photoinduced Charge Transfer in Semiconductor Quantum Dots-Polymer Hybrid Solar Cells

Research Team: Ponnusamy Nachimuthu, Ajay Karakoti, Shail Sanghavi, Theva Thevuthasan (PNNL)
Key Collaborators: David Shuh (LBNL)

Purpose

Develop a novel integration of molecular imaging and spectroscopy capabilities that will advance the fundamental understanding of the photo-induced charge transfer in hybrid solar cells.

In particular, study the concentration and size-dependent distribution of the CdSe quantum dots in conductive polymer films (P3HT), the chemical and electronic structure interactions and their influence on the photoinduced charge transfer and the efficiency of the hybrid solar cells.

Expected Outcomes

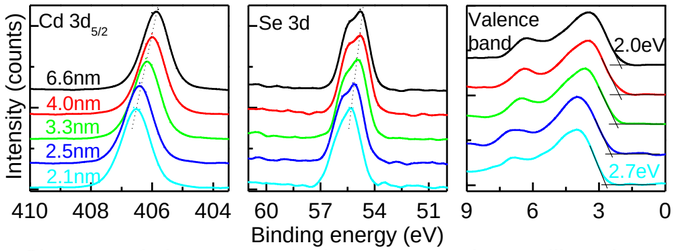
1. Obtain valuable insights into the complex interfaces of hybrid solar cell devices that employ nanoscale materials and advance the technology through fundamental study.

2. Expand the use of He ion and x-ray based imaging techniques with spectroscopic techniques to resolve other important technological problems at PNNL.

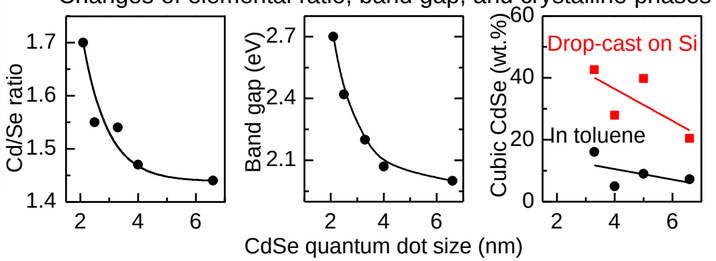
Progress

Establishing size and structure-property relationship

X-ray photoelectron spectroscopy



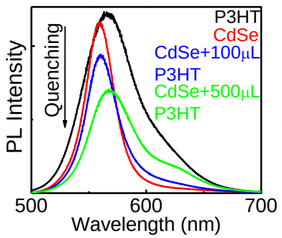
Changes of elemental ratio, band gap, and crystalline phases



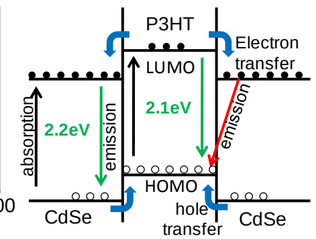
Binding energies of core levels and the valence band shift to higher energies with decreasing size showing quantum confinement along with changes in Cd/Se ratios, band gaps, and crystalline phases.

Incorporating CdSe in P3HT – band changes and agglomeration

PL emission in toluene

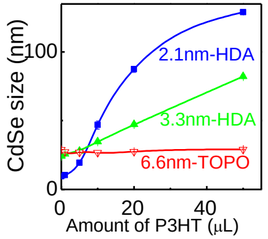


Energy diagram

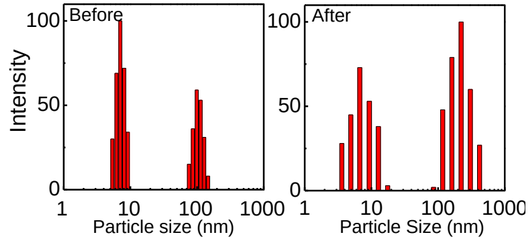


Addition of P3HT into CdSe quenches the fluorescence; a new band emerges from the recombination.

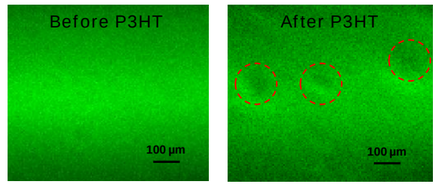
Agglomeration with P3HT



Size distribution of CdSe with P3HT addition



Soft x-ray imaging of CdSe drop-cast on Si



Incorporating CdSe quantum dots in P3HT matrices increases the agglomeration that changes with size.

Publications and Presentations

Probing the size-induced electronic structures of CdSe quantum dots, Ajay Karakoti et al., M & M Conference, Nashville, TN, Aug 2011 and AVS International Symposium, Nashville, TN, Oct 2011

Probing the electronic and in situ crystalline structures of CdSe quantum dots, Ajay Karakoti et al., manuscript submitted for publication, July 2011

Pacific Northwest NATIONAL LABORATORY
Proudly Operated by Battelle Since 1965