Stony Brook University
The Graduate School

Doctoral Defense Announcement

Abstract

Nanoscale Spatial Inhomogeneity in Photovoltaic Devices

By

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A substantial challenge in the development of optoelectronic devices is the inherent non-uniformity in semi-crystalline and polycrystalline photoactive materials. The focus of this work is to understand and evaluate the impact of specific non-uniformities in organic and inorganic materials used in optoelectronic devices, and present strategies for the development of novel architectures where they can be beneficial. We focus on materials in two regimes: a) materials with a small dielectric function, where electron-hole pairs, or excitons have radii on the order of the size of the unit cell (Frenkel excitons), and b) materials with a larger dielectric function, where excitons have radii larger than the lattice spacing (Wannier excitons). In the first regime, we focus on organic electronic materials specifically poly-(3 hexylthiophene), a conjugated semiconducting polymer, and [6,6]-phenyl-C-61-butyric acid methyl ester, an electron accepting fullerene derivative. We measure the donor-acceptor volume fraction and the inter-chain disorder in thin-films as the film thickness approaches the confinement limit (< 20nm), using variable angle spectroscopic ellipsometry and near-edge X-ray absorption fine structure spectroscopy. We also investigate the effect of confinement on the coherence length and the crystalline microstructure of the polymer using grazing incidence wide angle X-ray scattering. As the film thickness approaches the confinement regime, the films became less phase segregated and the polymer component formed less disordered smaller crystallites. In the second regime, we focus on understanding the recombination mechanism in polycrystalline $Cu(In_{1-x}Ga_x)Se_2$ due to material compositional inhomogeneity. We measure the charge transport behavior as a function of temperature of few-grain regions using lithographically defined electrical contacts and correlate these measurements with energy dispersive X-ray spectroscopy and aberration corrected transmission electron microscopy. We find that local regions with a higher fraction of copper-rich grains showed enhanced interfacial recombination whereas regions with a higher fraction of copper-poor grains show standard bulk limited recombination. Finally, we present novel architectures where material non-uniformities are used beneficially: a) we demonstrate strong (2.11×10^{13} e/cm^2), robust, and spontaneous graphene n-doping on polycrystalline $Cu(In_{1-x}Ga_x)Se_2$ due to surface-transfer doping from sodium; b) we demonstrate broadband tunable antireflection using densely packed silicon nanotextures, comprising a surface layer whose optical properties differ substantially from those of the bulk, providing the key to improved performance.

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