



Global Climate & Energy Project STANFORD UNIVERSITY

Molecular Solar Cells

Investigator

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Objective

This project aims to create a high-efficiency, molecule-based organic photovoltaic cell. Novel molecular semiconductors will be engineered to increase photon absorption in the visible and near-infrared (NIR) spectral ranges, and multiple deposition techniques and post-treatment technologies will be investigated to optimize the nanoscale morphology of random and ordered bulk heterojunctions. This research includes the study of molecular nanocrystals as a way to enhance exciton diffusion and charge transport. Degradation mechanisms and cell lifetime will be studied and measured under ultrahigh vacuum conditions. The use of intrinsically stable pigment molecules may result in cell lifetimes greater than ten years under solar illumination.

Background

Photovoltaic devices based on organic semiconductor materials that can be deposited in roll-to-roll vacuum coaters are attracting increasing interest because of their potential to provide efficient and low-cost alternatives to traditional solar cells. Over the last ten years, laboratory cell efficiency increased steadily to current values of approximately 6%. However, new routes need to be explored to further increase efficiency and lifetime in order for this technology to compete with inorganic thin films.

The purpose of this project is to develop efficient and durable organic-based devices using novel molecular semiconductor materials, deposition techniques, and bulk heterojunction architectures. Specifically, all fundamental processes governing the conversion of solar photons into electricity (see Figure 1) will be studied and optimized as follows: (1) Photon absorption: engineer novel active organic materials to enhance absorption in the NIR spectral range and design multijunction cells to optimize solar spectrum coverage. (2) Exciton diffusion: enhance exciton diffusion length by controlling the morphology of the film during deposition and post-treatment phases. This task includes the investigation of molecular packing, submicron molecular single crystals, and donor-acceptor interface geometry. Different device architectures will be explored to determine the optimal device structure. (3) Charge transfer and separation: optimize the molecular parameters

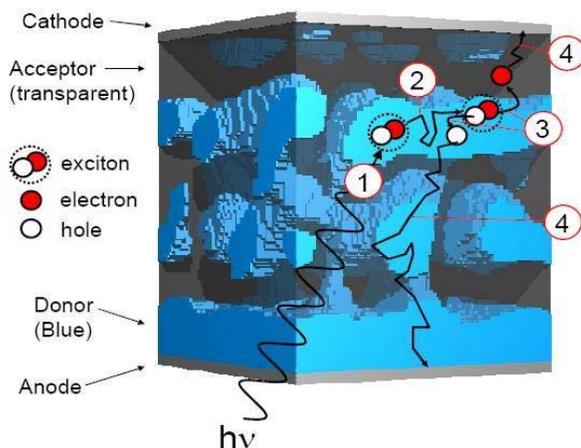


Figure 1: Schematic of a bulk heterojunction organic solar cell and illustration of the fundamental processes of the photon-to-electricity energy conversion.

and donor-acceptor interface energetics (namely, the energy level offset) against charge transfer efficiency. (4) Charge transport and collection: investigate the influence of nanoscale morphology on carrier mobility in different cell structures in order to optimize charge transport to the electrodes.

Approach

Novel molecular semiconductors will be synthesized and engineered to enhance photon absorption in the visible and NIR spectra and to optimize charge-transfer processes at the donor-acceptor interface. The first candidate for this application is copper phthalocyanine (CuPc), which was selected due to its strong optical absorption ($1-2 \times 10^5 \text{cm}^{-1}$ in solid state), high intrinsic stability (up to 350°C in air), and low cost. Non-sublimable molecules such as very large aromatic core molecules will be explored for sub-1eV bandgaps.

A variety of deposition techniques will be studied to generate different film morphologies and to deposit and combine materials that cannot be spin-coated or sublimed, such as large molecules with low bandgaps. Novel techniques to be explored here include organic vapor phase deposition (OVPD) that allows the growth of ordered CuPc nanowire structures (see Figure 2), the aerosol deposition (AD) method, which allows the mixture of large molecules with (in-)organic nanocrystals and the easy growth of multilayer coatings, and the supercritical deposition (SD) technique that, like AD, makes it possible to control the crystal formation of the active layers. The

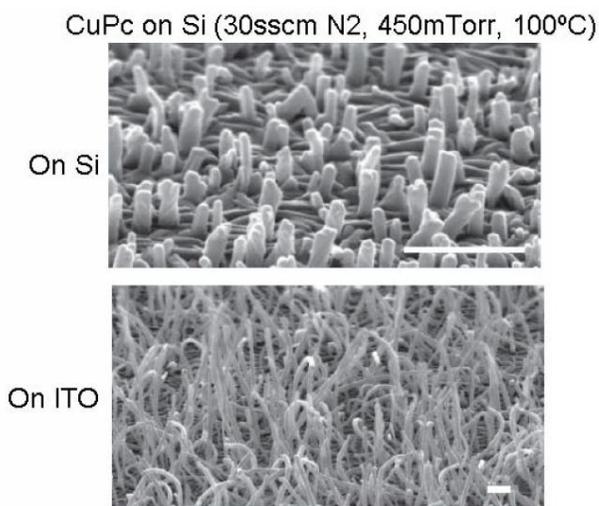


Figure 2: Nanowires of CuPc grown on Si and ITO using OVPD [1].

above deposition techniques will be used to build and optimize the morphology of several devices including disordered nanostructured cells (random bulk heterojunctions grown by co-deposition of donor and acceptor materials), ordered nanowire structures, and nanocrystal-based cells (using both inorganic and molecular nanocrystals). Energy and charge transport in all these structures will be studied experimentally using electron-spin resonance-based imaging techniques on the nanometer scale, and modeled with simulation tools that account for the correlated motion of excitons, electrons, and holes in a nanostructured device. Finally, multijunction cells will be built using thin metal particle-based films as ohmic contacts between subcells. It is calculated that 30% conversion efficiency may be reached in a six-cell stack with an energy level offset of 0.5eV. Device lifetime and the nature of the degradation mechanisms will be studied in ultrahigh vacuum under accelerated conditions. Of particular interest are the effects of temperature, illumination intensity, and contaminants.

References

1. F. Yang, M. Shtein, S.R. Forrest, *Nature Materials* 4, 37 (2005)