Project 03: Highly-Efficient Low-Cost Polymeric Solar Cells
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Harvesting energy directly from sunlight using solar cells is a very important way to address growing global energy needs with a renewable resource while minimizing detrimental effects on the environment by reducing greenhouse gas emissions. In fact, photovoltaic cells are considered by many scientists as the most promising renewable, clean, and portable source of energy of the future. However the high manufacturing cost of current crystalline Silicon solar cells prohibits this technology from having significant impact on global energy production. During the past 10 years, novel classes of synthetic conjugated polymers (e.g. polythiophenes, polyphenylenevinylenes, polyfluorenes, etc.) have emerged as potential alternatives to the relatively expensive current technologies based on Silicon and other materials. For instance, they have the potential to be flexible and manufactured over large areas using wet-processing or printing techniques which will reduce costs compared with traditional photovoltaic cells.[1,2,3]

Various combinations using light-absorbing conjugated polymers as a donor and organic or inorganic semiconductors as an acceptor have been developed to build bulk heterojunction (BHJ) solar cells. In these cells, the composite active layer is inserted between two electrodes with different work functions: a transparent front electrode consisting of indium tin oxide (ITO) for hole collection and a metal back electrode for electron collection. In such configurations, power conversion efficiencies about 5-6 % under simulated AM 1.5 illumination were recently obtained. However, this technology still faces issues of relatively low device efficiency and short useable lifetime as compared to Silicon-based solar cells. Some of the major factors limiting the power conversion efficiency in organic solar cells are :

- Most organic semiconductor materials have poor absorption for red (low energy) photons, which represent a significant fraction of the energy in the solar spectrum, leading to low power conversion efficiency in organic solar cells.
- The exciton diffusion lengths in organic materials are only around 5-10 nm. In order to dissociate the excitons into charge carriers before recombination, a charge separation interface (heterojunction) should be in close proximity to the exciton generation site. In traditional heterojunction devices, this means using a very thin absorbing layer and consequently, the total light absorbed will be significantly reduced.
- Organic semiconductor materials have much lower charge carrier mobilities (10^{-7}-1 cm^2/Vs) as compared to traditional semiconductors (1-10^4 cm^2/Vs), leading to high series resistance and low fill factors, directly affecting the final power conversion efficiency.
- In order to obtain maximum photocurrent, it is necessary to extract both types of charge carriers efficiently. Moreover, most organic semiconductors have a huge difference between their hole and electron mobilities, leading to imbalanced charge transport of hole current and electron current, thus limiting the power conversion efficiency.

A significant amount of research effort has been therefore dedicated to the synthesis of low energy gap polymers for better light absorption[4,5] and to the design and engineering of different types of bulk heterojunctions. The BHJ structure involves mixing the p- and n-type materials and relying on the intrinsic tendency of polymer materials to phase-separate on a nanometer scale to form a bi-continuous, interpenetrating p- and n-type network. This minimizes the average distance between the light absorber and the heterojunction for efficient harvest of excitons, while simultaneously allowing thicker films for increased light absorption. Investigations of new types of electrodes have also recently received a great deal of attention.[6]

In this project, we have assembled a cross-disciplinary research team from 3 universities to address these problems. First, the project will benefit from theoretical support to help understand the electronic interactions between the different constituents of organic solar cells. Alignment of energy levels is

critical to promote charge transfer at the interfaces. With the help of *ab initio* calculations[7,8] it will be possible to simulate the interaction between different parts of the system (surface/ polymer or polymer/ C_{60})[9] and determine the energy levels and wave functions involved in the charge transfer process. For example, it will enable us to obtain an understanding at the microscopic level of the role of the functionalized surface in helping to promote charge transfer. Such calculations can be carried out using a standard approach within the framework of density-functional theory (DFT). However, it might be necessary to obtain more accurate values of the energy levels than provided by DFT which is known to underestimate the band gap with certain functionals. The use of an approach based upon a Green's function method, known in the community as the GW method[10] is clearly the favoured approach in this case but it is restricted to smaller systems than DFT. M. Côté's group (U. de Montréal) has the goal of improving the applicability of the GW method to large systems, a development which will be done through a project to design low band gap polymers (Project 5.4.2). We will then use their development to help characterize the produced devices.

The team of M. Leclerc will prepare in relatively large quantities different conjugated polymers developed in parallel with the research project 5.4.2. These new conjugated polymers should exhibit various HOMO and LUMO energy levels together with variable bandgaps. These hole-transporting polymeric donors should be blended with different fullerene derivatives to yield different types of bulk heterojunctions. An undergraduate student will scale-up all new polymers developed by the research teams of S. Holdcroft and M. Leclerc. A Master's student will also work on the synthesis of new functionalized fullerene derivatives to modify their LUMO levels and their electron mobility. Optimization of the electronic properties is another method to increase the open circuit voltage and therefore, the overall efficiency of the polymeric solar cell.

The new polymeric materials and fullerene derivatives will be sent to J. Buriak (U. of Alberta and the National Institute for Nanotechnology) where their hole and electron mobilities will be evaluated by a variety of means, including time-of-flight (ToF), electrochemistry, and other methods. Various approaches will be pursued to produce nano-structured polymeric morphologies, including incorporation of functional nanoparticles and self-assembling polymeric templating agents. These materials will be characterized via atomic force microscopy (AFM), scanning electron microscopy (SEM) depth profiling by X-ray photoelectron spectroscopy (XPS), mass spectrometry (ToF-SIMS), scanning Auger microscopy, and others. In parallel, the J. Buriak research team will push the development of new modified electrodes (both transparent conducting electrodes, and reflective metallic electrodes) that lead to better charge extraction. The surface chemistry of these materials will be modulated to control work function, wetting behaviour, and covalent connectivity with the overlaying conducting organic media.

On the basis of this information, various photovoltaic devices will be fabricated and evaluated in the laboratory of J. Buriak. This will involve a full-spectrum solar simulator for electrical characterization, as well as spectrally resolved external quantum efficiency equipment. Different morphologies and device configurations will be tested through a variety of thin film deposition techniques, including spin-coating, dip coating, spray coating, inkjet printing and doctor blading. Also, the utilization of various processing additives (surfactants, compatibilizers, etc.) will be investigated, as will the insertion of buffer layers to act as exciton blockers. Electrical stability of completed devices will also be investigated in a variety of environments (humidity, temperature, oxygen levels). The work will first focus on the development of high-efficiency single layer devices, and will branch out to tandem cells to further push the efficiency higher. Through a collaboration with A. Heeger (U. of California, Santa Barbara), we will develop optimized polymeric solar cells.

At the end of this project, it is anticipated that new highly efficient and low cost polymeric solar cells will be obtained through optimization of polymeric donors, fullerene acceptors, modified electrodes, and processing techniques. For instance, an efficiency of 7.0-7.5% is targeted for the end of the third year and values up to 9% are anticipated by the end of this 5-year project.

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