Project 02: Improving Organic Solar Cell Efficiency Using Low Band Gap Polymers and Tandem Devices

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The advantages of organic solar cells are their light weight, flexibility and low processing cost. However, their usefulness is limited due to their relatively low power conversion efficiency. Presently, the best organic solar cells show efficiencies of around 6%[1,2] whereas polycrystalline Silicon devices reach an efficiency of 15%. It is therefore essential to improve the efficiency of organic solar cells, which can only be achieved by designing new organic materials.

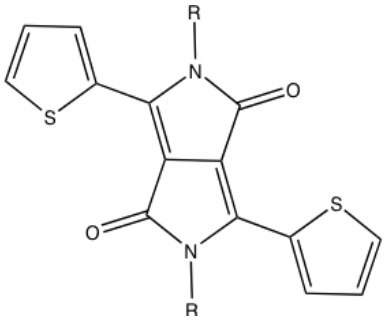


Fig. 5: Diketo-pyrrolo-pyrrole molecule with thiophene on each side.

The objective of this project is to make new polymers that will be used in organic devices. To achieve this objective we combine the expertise of two synthesis groups, those of M. Leclerc at Laval and S. Holdcroft at Simon Fraser, and the theoretical group of M. Côté at the U. de Montréal. This collaboration will establish a synergy between these complementary approaches that will result in faster development of new polymers.

To reach our goal, we can identify the desirable properties of these new polymers:

- Low band gap to harvest more of the solar spectrum
- High charge mobility
- High ionization potential to improve stability
- High electronic affinity to allow electron conduction
- Good solubility properties suitable for photovoltaic devices.

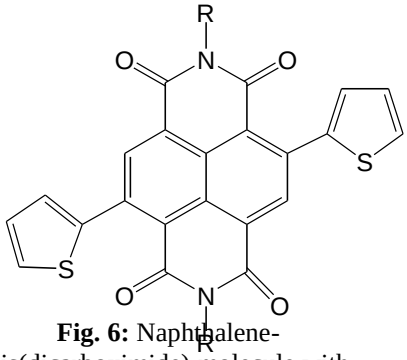


Fig. 6: Naphthalene-bis(dicarboximide) molecule with thiophene on each side.

The long-term stability of organic solar cells is always an issue. To improve the stability, we must design polymers with low HOMO energy, and high ionization potential, preferably lower than 5 eV below the vacuum level such that they will not oxidize. One way to achieve this goal is to include nitrogen atoms within the polymer backbone. For example, polymers made with the molecules shown in Figs. 5 and 6 show HOMO of 5.5 eV. Furthermore, these polymers demonstrate charge mobilities on the order of 0.1 cm^2/Vs, a very high value for organic polymers[3,4]. An additional advantage of these polymers is their low LUMO energy, i.e. high electron affinity, of around 4 eV, a value close to the LUMO value of PCBM. These polymers could be used as electron carriers in solar cells replacing PCBM and thus helping to keep the cost of these devices as low as possible.

The group of M. Leclerc will integrate these molecules and other nitrogen rich molecules in a copolymer synthesis process with heterofluorene, see Fig. 7, that has proven to be successful in making efficient polymers for photovoltaic applications[5]. This route offers a wide range of possibilities where X can be any of the elements C, N, B, Si or Ge and Y any of the molecules mentioned above. Different synthetic strategies will be involved to get well-defined and pure homopolymers and copolymers.

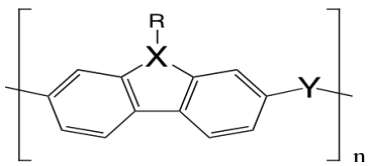


Fig. 7: General copolymer structure with heterofluorene.

Clearly the synthesis of all the possibilities enumerated could take many years. In order to select only the most promising candidates, we will make use of *ab initio* calculations of the electronic properties provided by M. Côté's group to help assess these polymers before the synthesis is done. Such collaboration between the experimental and theoretical efforts has been proved useful in previous analysis of polymers for photovoltaic applications.[6]

Calculations within density-functional theory (DFT) with the B3LYP functional provide a relatively fast way to determine the electronic and optical properties of polymer systems[7,8]. With such an approach, we will be able to assess the potential of all these novel polymers in a time frame of a few months. It also allows the quick evaluation of other ideas that might arise through our collaboration between the synthesis groups of M. Leclerc and S. Holdcroft and the theoretical group of M. Côté.

With the help of *ab initio* calculations it is possible to study the effects of modifications in the polymer structure to determine if the properties are improved. For example, the PCPDTBT polymer depicted in Fig. 8 has been used in solar cells with an efficiency of 5.5%.[9] Our calculations indicate that if nitrogen atoms are included in the atomic structure as shown in Fig. 9, it will result in a lower HOMO and LUMO by 0.4 eV as compared to the original PCPDTBT polymer. If such a polymer was to be used in devices with PCBM, it would be more stable and should result in an increased V_{OC} and thus a higher efficiency.

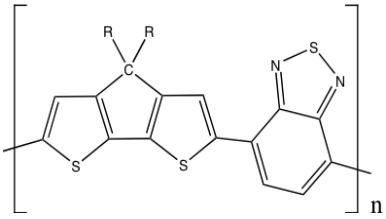


Fig. 8: PCPDTBT polymer

Determining electronic properties with DFT is useful to reveal the trends within a family of organic polymers. In order to obtain an accurate description of the optical properties and the positions of the HOMO and LUMO levels, other methods need to be used. A very precise approach is to use the GW method followed by the Bethe-Salpeter method that has proved useful for determining optical properties in polymers[10]. However, such a combination of approaches is very demanding in computational resources and only relatively small systems can be calculated. Recently, many developments[11,12]have been proposed to increase the system size studied by these approaches. It is our intention to adapt these developments and others in our computational tools so that we will be able to accurately address the polymers proposed in this project. Such calculations will take several weeks. As such, we will begin with a few selected systems which have been identified as promising by the more standard DFT approach.

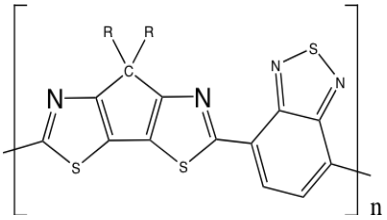


Fig. 9: A modified PCPDTBT polymer

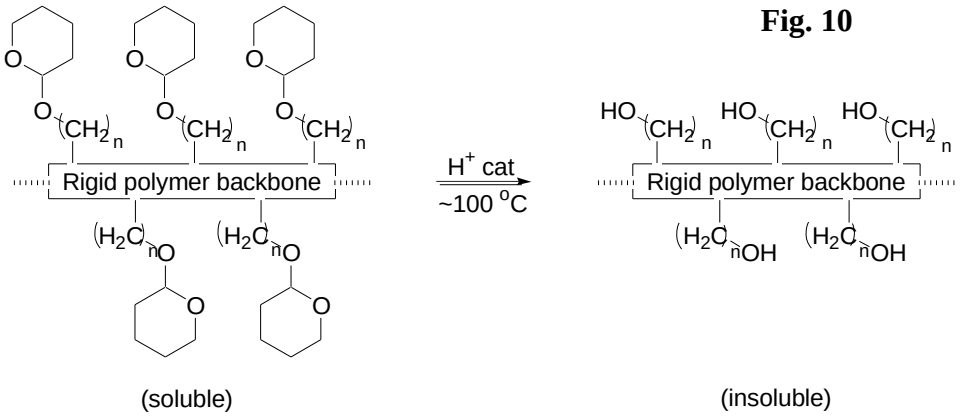
This synthesis strategy should yield polymers with energy gaps in the range of 1.0 to 1.5 eV which should be optimal for single active layer bulk heterojunction devices[13]. To reach efficiencies comparable to inorganic devices, other strategies will need to be explored. One strategy is to use a tandem design for the solar cell. According to the Shockley-Queisser limit, the efficiency for a single active layer device is 30% whereas the theoretical limit for a tandem design reaches 42%[14].

Several approaches for organic tandem cells have been reported over the past several years[15,16]. We favour an all solution-process approach in order to keep the cost low; however, this requires a judicious choice of solvent when preparing subsequent layers as to prevent disruption of the bottom cell while preparing the top cell. The use of polymers with thermocleavable substituents eliminates this criterion as thermal annealing following solution processing cleaves the solubilizing group generating an insoluble film. Thus preparation of the top cell would no longer disrupt the bottom cell.

To that end, the group of S. Holdcroft will study the synthesis of conjugated polymers bearing a tetrahydropyranyl (THP) substituent attached to the alkyl chain as the donor material for tandem solar cells. These polymers are soluble in common organic solvents and, following thin film preparation, the

THP group may be thermally or photochemically converted to a hydroxyl group by acid catalysis, as shown in Fig. 10, rendering the film insoluble[17,18,19,20]. Thus subsequent layers may be deposited regardless of solvent choice.

Fig. 10



With such an approach, we will then be able to combine the low band gap polymers developed in M. Leclerc's group with properly functionalized higher band gap polymers made in S. Holdcroft's group in tandem organic cells to harvest the solar spectrum optimally. Another critical component of a tandem solar cell is the metal contact between the two active layers. Different solutions have been proposed, i.e. Ag nanocrystals or TiO_x, but all involve inorganic materials. In this project, we will explore the use of a conducting nanotube layer[21] that will have the advantage of being an all organic process as well as retaining the flexibility of the device.

This research project should therefore lead to highly performing single and tandem polymeric solar cells. On the basis of present knowledge, 10% efficiency can be anticipated for single layer solar cells whereas efficiencies up to 15% could be achieved in a tandem configuration.

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