Bulk Heterojunction Organic Solar Cells utilizing a Benzothiadiazole-based Oligomer

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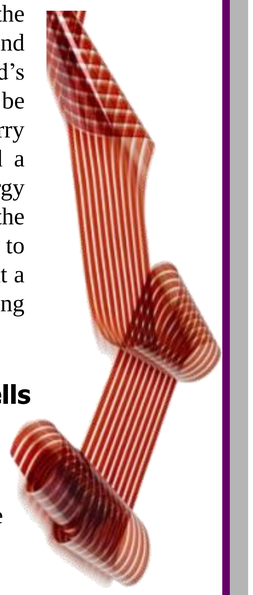
1 Why organic solar cells?

With predictions estimating that the reserves of oil, natural gas, and coal—historically three of the world's most prominent energy sources—will be scarce within the next 200 years, a flurry of research is being conducted to find a viable option to alleviate global energy concerns. One proposed solution, the organic solar cell, has the potential to convert solar energy into usable power at a commercially-feasible price point by using a thin film of conductive polymers.



Ink jet printed organic solar cell

Advantages over silicon solar cells

- Roll-to-roll manufacturing lowers costs through a faster rate of production
- Flexible substrates allow for coverage on a wider variety of surfaces
- Use of polymers allows for tuning of properties to optimize absorbance, band gap, etc.

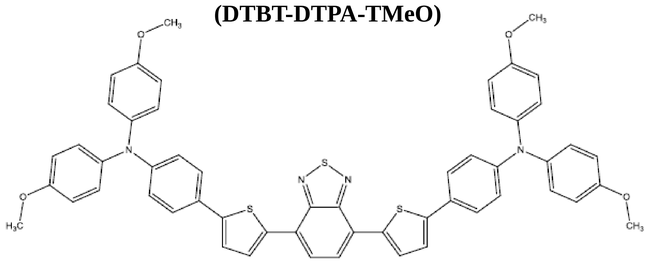
Still, organic photovoltaics (OPVs) must overcome a variety of challenges (limited absorbance, low and variable life expectancies, and efficiencies roughly **50%** of those of silicon solar cells) before they are suitable for widespread use; until then, traditional solar cells, which have issues of their own, will remain the dominant solar energy provider and the world will continue to rely largely on fossil fuels.

Research Objective

Our work centered on the development of organic solar cell devices utilizing a new oligomer blend spin-coated as a bulk heterojunction thin film. We wanted to improve the performance of OPVs and see if this oligomer could be used as a potential substitute for known donor materials. Additionally, the effects of annealing on charge transport were examined.

2 What is the molecule?

Tertmethoxy Di-triphenylamine Di-thiophene-benzothiadiazole (DTBT-DTPA-TMeO)



Molecular Formula: $H_{42}C_{54}O_4N_4S_3$ **Molecular mass**: 906 amu

- Solution processable oligomer; allows for spin coating
- Synthesized donor-acceptor-donor (D-A-D) configuration
  - Middle benzothiadiazole acts as an electron acceptor
  - Outer thiophene-triphenylamine moieties are donors
- Lowers bandgap (E_g) to a theoretical value of **1.93 eV**
  - Value measured as **1.81 eV** [1]
- Absorbance peaks at around **380 nm & 550 nm** [1]
- Thermally stable with a decomposition temperature ~ **400°C**

3 How is the blend made?

- Equal parts DTBT-DTPA-TMeO and PCBM (1:1 by weight)
- Add chloroform to form blend solution
  - 5 mg/mL concentration
- Mix in ultrasonic bath and water bath (50°C)
  - Aids with dissolving process; particles that remain in solution can cause film defects

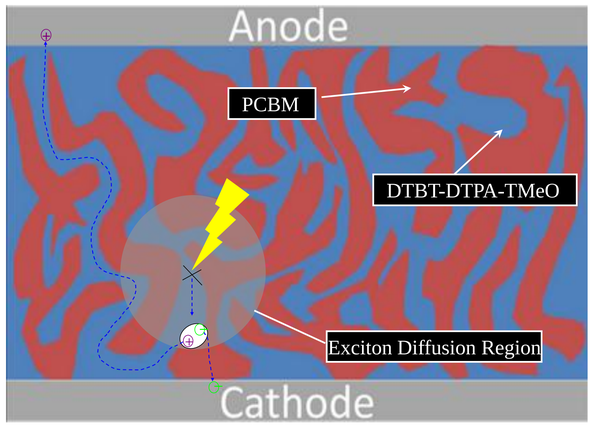
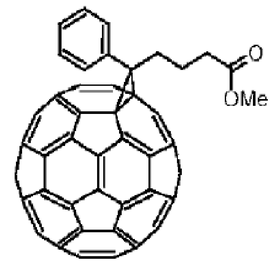


Figure 1: Model of an exciton's lifespan within the bulk heterojunction layer of the cell



PCBM
(1-(3-methoxycarbonyl) propyl-1-phenyl[6,6]C_{61})

Blend Purpose

Oligomer: Electron donor **PCBM**: Electron acceptor

- High differences in the electron affinities of the two molecules overcome exciton attraction forces
  - Happens at molecular boundaries
- Mixing the donor and acceptor molecules in a bulk heterojunction layer promotes electron transfer
  - Exciton diffusion length (L_D): Average distance an exciton can travel through a medium; intimate mixing of the blend ensures that the distance from a generated exciton to a dissociation interface is less than L_D.

4 Experimental Procedure

- Clean indium tin oxide (ITO) glass substrate
  - Detergent, pure water, acetone, boiling 2-propanol
  - Ultrasonic bath while in each solution
  - Blow dry with inert gas (argon)
- Vapor deposit a molybdenum trioxide layer (lower hole barrier)
  - All vapor deposition at 10^{-6} torr
- Spin coat a thin film of the blend solution (~3500 rpm)
- Vapor deposit a bathocuproine (BCP) layer (lower electron barrier)
- Vapor deposit an aluminum cathode layer
  - Keep a low, steady rate (~2Å/sec) to avoid overheating

Figure 2: 9 OPV devices

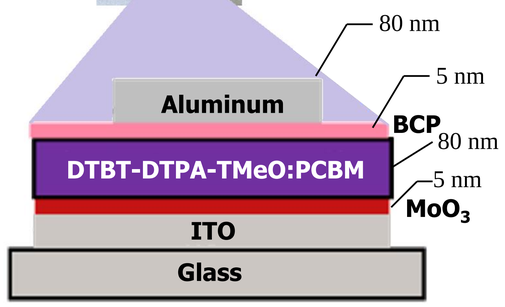


Figure 3: Cross-section showing layer thickness in an OPV device

5 How is the quality of the film?

- AFM imaging was used to view the surface morphology and microstructure of the spin-cast blend film on ITO/MoO_3
- Ideal film would have very few defects (pinholes, large features); virtually homogenous mix of the two molecules
  - Ensures proper transfer of electrons, high charge mobility, and high cell performance
- Experimental film shown in Figure 4b displays pinholes and features caused by the colloidal nature of the mixture
  - Particles cause "flare-like" effects in the film (see Figure 5)
  - Film thickness roughly 50% of desired value
- Plain ITO glass is shown (Figure 4a) to demonstrate the effectiveness of the cleaning procedure
  - Eliminated virtually all dust & organic material

Figure 5: Flare effects in a spin-coated thin film, leads to areas of uneven coverage (white)

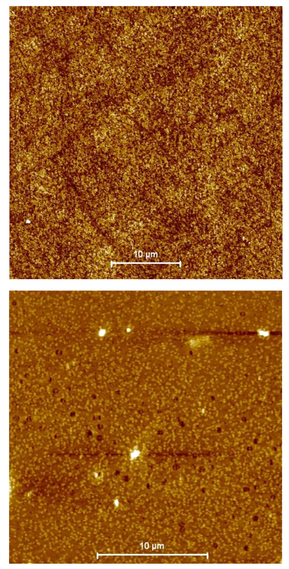


Figure 4: AFM images a) Clean ITO glass b) 40 nm thick film of blend solution on ITO

6 What were the results?

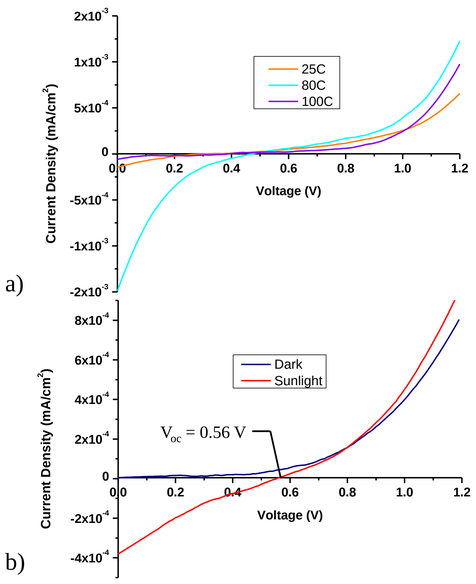


Figure 6: J-V characteristics a) Temperature dependence without BCP b) with BCP at room temperature

- Clear temperature dependence (improvement of film quality; e.g. less solvent, smoother surface, intimate contact between polymers); results improve until ≈ 100°C when annealing begins to damage the film

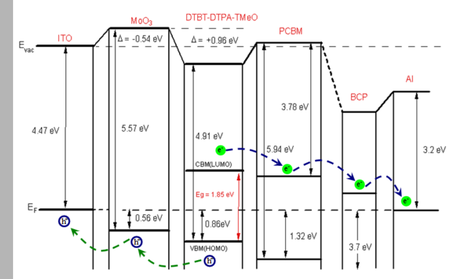


Figure 7: Energy band diagram for the OPV

- E_g = 1.85 eV
- HOMO = -4.91 eV
- LUMO = HOMO + E_g = -3.06 eV

	No BCP, Room Temp.	No BCP, 80°C	No BCP, 100°C	BCP, Room Temp.
V_{OC}	0.37 V	0.47 V	0.40 V	0.56 V
I_{SC}	$1.06 \cdot 10^{-9}$ A	$8.28 \cdot 10^{-9}$ A	$7.91 \cdot 10^{-8}$ A	$2.83 \cdot 10^{-8}$ A

Table 1: LabView Output

- Very low values of current; generated excitons appear to get trapped in film defects

7 Conclusions & Future Steps

- DTBT-DTPA-TMeO can be applied to glass substrates via spin coating methods for use in OPVs
- V_{OC} values similar to other donor materials were achieved
- Temperature affects the surface morphology of the film
- A bathocuproine layer appears to increase the V_{OC} (+0.09 V)

Work is currently in progress to achieve a homogenous surface morphology free of defects; it is likely that performance would be improved and results would be more consistent. Also, further tests to determine the optimum annealing temperature (around 80°C) must be conducted. In addition, experiments must be done to determine the longevity of the blend.

Acknowledgements

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Yilin Li (WSU) was responsible for developing the oligomer

Candy Mercado (WSU) was instrumental in testing the devices

[1] Measurements were based on REU work done by Ross Kerner (2011)