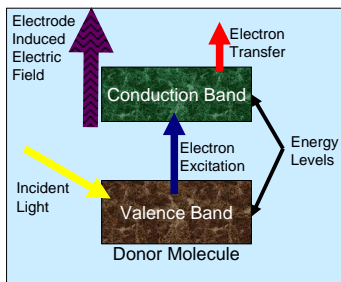


Organic Solar Cells from Functionalized Donor-Acceptor Molecules

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Introduction



- Organic solar cells use polymers instead of metals or silicon to produce electricity from photons.
- Polymers are generally considered to be insulators, but a certain kind called conjugated polymers can transmit electrons with resistances very close to that of metals.
- Several of these electron donating polymers are known to photoluminesce (a process in which an electron is promoted into the conduction band) when illuminated.
- In photovoltaic devices, donor polymers are paired with acceptor molecules. These acceptor molecules must be chosen such that the electrons in the conduction band are transferred from the donor molecule before they can relax from the excited state.
- Advantages of these solar cells is that they are relatively easy to produce on a manufacturing scale by methods like spin coating, dip coating, or a roll to roll process.

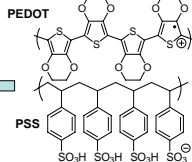
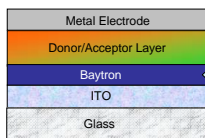
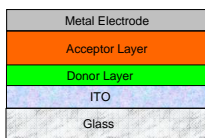
General Device Structures

Bilayer Cells

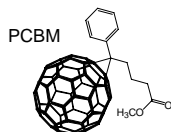
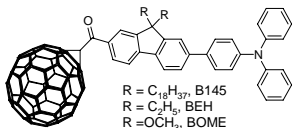
- Bilayer organic photovoltaic cells are made by depositing donor and acceptor layers directly over one another.
- Only about 10% of the thickness of the contacting donor and acceptor layers will experience electron transfer.
- Thus, device efficiency is relatively low with this fabrication process.

Bulk Heterojunction Cells

- Similar to bilayer cells except the donor and acceptor are blended in a single layer.
- This design increases the surface contact between the donor and acceptor, significantly enhancing electron transfer, and increasing the efficiency compared to bilayer devices.
- Baytron is a dispersion of the conjugated polymer PEDOT and the polyanion, PSS.
- The Baytron layer smoothes out the electrode, helping to eliminate shorts.



Single Molecule Donor/Acceptor Structure



- All of the donor-acceptor molecules are based on a functionalized Bucky Ball (C₆₀) nanoparticle called PCBM.
- C₆₀ is known to be a good electron acceptor but is nearly insoluble.
- The PCBM derivative is capable of being formed into more complex molecules that may have a higher solubility.

- In this design, a molecule is tailored to incorporate donor and acceptor functionalities within a single molecule. This will ensure that no excited electrons are allowed to relax back into their ground state, and 100% electron transfer is possible.
- The molecules (B-145, B-EH, B-OME) are dissolved into chloroform to create a 1% (by mass) solution that is spun onto ITO in the same fashion as a bulk heterojunction cell.

Device Fabrication



- While ITO is available commercially on glass slides, the Baytron and active polymer must be applied from solution.
- In this application, spin coating was used to produce a uniform film thickness from 50-200nm.

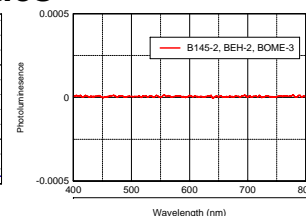
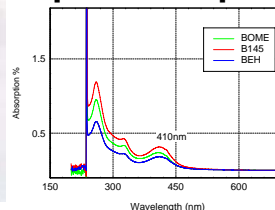
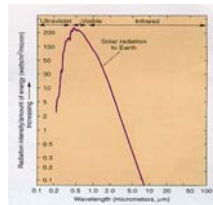


- Device performance has been shown to decrease rapidly when exposed to O₂ and H₂O.
- Thus, all processes involving the active polymer layer are done in a nitrogen environment glove box.



- To complete the device an aluminum electrode must be applied.
- In order to achieve maximum surface contact with the active layer film the aluminum is thermally evaporated to a thickness of 100-200nm

Optical Properties

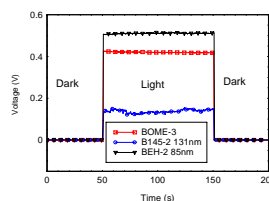


- Solar radiation intensity is maximized in the visible light range.
- A power of 100mW/cm² is transmitted.

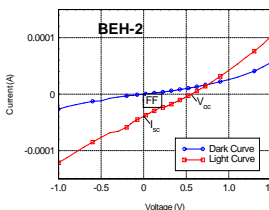
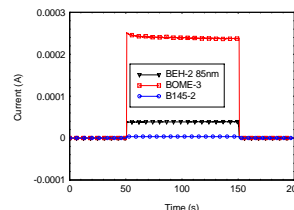
- The three molecules have an absorbance peak in this range at 410nm.
- This is where the greatest amount of power will be produced under solar light.

- Total quenching of photoluminescence was observed upon illumination at 410nm for all molecules, demonstrating complete electron transfer from donor to acceptor within the molecules.

Device Performance



- Testing of devices with time helps to determine their photovoltaic parameters.
- An erratic voltage or low current shows a device that will have a low performance.



- Current-voltage (I-V) plots are measured in the dark and under solar simulated illumination to measure diode behavior.
- The open-circuit voltage (V_{oc}) and short-circuit current (I_{sc}) are the points at which the light I-V intersects the abscissa and ordinate, respectively.

- The Fill Factor (FF) gives an indication of how close the device operates to an ideal diode.

$$FF = \frac{V_{mpp} I_{mpp}}{V_{oc} I_{sc}} = \frac{P_{max}}{V_{oc} I_{sc}}$$

- The power conversion efficiency (η) is simply the power of the sun's incident photons divided by the measured power output of the device.

$$\eta = \frac{P_{out}}{P_{in}} = FF \frac{V_{oc} I_{sc}}{P_{in}}$$

Molecule	Fill Factor	Maximum Efficiency
B145	0.253	0.0033%
BEH	0.263	0.0354%
BOME	0.295	0.184%

Conclusions

- A photovoltaic effect was observed for all three molecules under solar simulated irradiation.
- BOME, the molecule with the smallest and most polar R groups, showed the best device performance with the highest power conversion efficiency.

Future Research

Current Materials

- Conduction of a more thorough composition and thickness study of devices.
- New fabrication and testing of devices spun from solutions based on different solvents such as THF or Chlorobenzene.
- Analysis of device degradation processes under both inert and ambient conditions.

Second Generation Molecules

- Synthesis of new molecules with a larger absorption cross-section through the visible range of the solar spectrum.
- Changing the R group structure to allow for greater solubility in a broader range of solvents to simplify fabrication.
- Incorporation of new acceptor groups bonded to the chromophore for greater electron transfer.