Organic Photovoltaics using Novel Pentacene Derivatives

PhD Thesis Defense
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 collaborators

thesis motivation and goals

organic solar cells
  • device overview
  • design, fabrication and characterization
  • simulation findings

results and discussion

conclusions

future work and suggestions
Collaborators

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Thesis Motivation

The background

- Limited fossil fuel and environmental impact
- **Renewable sources of energy**
  - Wind, hydro, biomass, **solar** etc.
- **Solar cells types**
  - **Crystalline silicon devices**
    - c-Si and poly-Si
  - **Thin film devices**
    - GaAs, CdTe, DSSC, QDSC, **OSC**
• Photovoltaic technology and development (2012)
Photovoltaic Manufacturing: Present and Future

Projected convergence of the cost of electricity produced by PV and the grid prices,
Organic photovoltaic (OPV) cell’s benefits

- Organic semiconductors chemically synthesizable
- Less environmental pollution
- Low manufacturing cost
- Can be made flexible
- Can be made almost transparent to be used as window glass
- Solution processable
  
  (inkjet printing, roll-to-roll, doctor blade and Spin coating)
### Selected Efficiency Table for OPV cells (literature)

<table>
<thead>
<tr>
<th>Active layers</th>
<th>Type</th>
<th>Efficiency</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>P3HT: PCBM</td>
<td>Bulk heterojunction</td>
<td>4.7 %</td>
<td>Organic electronics, Vol. 12(2), 257 (2011)</td>
</tr>
<tr>
<td>CuPc/C₆₀</td>
<td>Bilayer</td>
<td>3.6 %</td>
<td>Appl. Phys. Lett. 79(1), 126 (2001)</td>
</tr>
<tr>
<td>Pentacene/C₆₀</td>
<td>Bilayer</td>
<td>2.8 %</td>
<td>J. Appl. Phy. 97, 103706 (2005)</td>
</tr>
</tbody>
</table>

P3HT - Poly(3-hexylthiophene); PCBM - Phenyl C₆₁ butyric acid methyl ester
MEH-PPV - Poly[2-methoxy-5-(2-ethylhexyloxy)-1,4-phenylenevinylene]
CuPc – Copper (II) phthalocyanine;
Statement of the Problem

• Power conversion efficiency (PCE) above 15% is required for commercial production of OPV cells.

• New organic semiconductor materials needed to be explored

• New materials should be solution processable or should be thermally evaporated

• They should be stable

• Optimum mobilities of charge carriers in photoactive layers need to be determined

• Optimum thicknesses of organic photoactive layers need to be found
**Contribution of this Thesis**

- Designed, fabricated and characterized OPV cells using following new pentacene derivatives:
  - Water Soluble Pentacene (WSP)
  - 5,6,7-trithiapentacene-13-one (TTPO)
  - C_{60} adduct of 6,13-bis(decylthio)pentacene (BC_{60}DTP)

- Simulation findings:
  - A new model developed for more accurate calculation of the electric field at the donor-acceptor interface
  - Determined optimal mobilities of charge carriers in active layers
  - Determined optimal layer thicknesses
  - Explored the effect of increased mobilities on efficiency
Organic Photovoltaics (OPV)

Device structures

(a) Single layer device (b) Bilayer or planar device and (c) Bulk heterojunction device
OPV - principle of operation

(a) Bilayer cell (b) Bulk heterojunction (BHJ) cell; (c) Energy band diagram of the device
Operational steps and loss mechanisms

- Photon absorption
- Exciton creation
- Exciton diffusion
- Charge separation
- Charge transport
- Charge collection

Loss mechanisms:
- Reflection ($I_L$)
- Transmission ($I_L$)
- Recombination of excitons after creation and during diffusion ($I_0$)
- Recombination of excitons when no charge separation ($I_0$)
- Recombination of charges ($R_{sh}$)
- Limited mobility ($R_s$)
- Recombination near electrodes ($R_{sh2}$)
- Barrier height ($R_s, I_o$)

Operational mechanism → Incident photons, I → Photocurrent
 Operational modes

Metal-insulator-metal band diagram under (a) short circuit (b) open circuit (c) reverse bias and (d) forward bias

Current-voltage curve of an OPV cell (dotted: dark current; solid: illuminated current). (a) short circuit (b) open circuit (c) reverse bias (d) forward bias
Device parameters

Equivalent circuit diagram for a PV cell

Output current:

\[ I = \frac{R_{sh}}{R_{sh} + R_s} \left[ \frac{V}{R_{sh}} - I_{ph} + I_0 \left( e^{\frac{q(V - IR_s)}{n k T}} - 1 \right) \right] \]

Shunt resistance: \( R_{sh} \approx \left[ \frac{dI}{dV} \right]_{V \approx 0}^{-1} \)

Series resistance: \( R_s \approx \left[ \frac{dI}{dV} \right]_{V \approx V_{OC}}^{-1} \)

Open circuit voltage:

\[ V_{OC} = |HOMO_D - LUMO_A|/q - 0.3 \text{ V} \]

Short circuit current \( I_{SC} = -I_{ph} \) (photocurrent)
Efficiencies and Fill-factor

- Internal quantum efficiency (relates to number of photons absorbed)
- External quantum efficiency or incident photon to converted electron ratio (EQE or IPCE):
  \[ IPCE = 1240 \frac{J_{SC}}{\lambda I_\lambda} \]
- Fill-factor: \( FF = \frac{I_m \times V_m}{I_{SC} \times V_{OC}} \)
- Power conversion efficiency (PCE):
  \[ \eta = \frac{I_m V_m}{P_{in}} = \frac{I_{SC} V_{OC} FF}{P_{in}} \]
Bilayer OPV using water soluble pentacene (WSP)

- WSP synthesized by Prof. Miller’s group at UNH, Durham
- The first water soluble pentacene derivative
- This acts as a donor
- Thin film coating of WSP was a challenge
- Fabricated OPV cell successfully and characterized

Schematic of WSP based OPV cell (left); Dektak profilometer reading of various layers (right)
Absorbance spectra of WSP in various solutions

Chemical structure of WSP or Potassium 3,3’-[(pentacene-6,13-diyl)bis(sulfanediyl)]dipropanoate

UV-Vis absorbance spectra for WSP in water, methanol and a buffer solution of pH 10

Substrate coating with WSP (10mg in 1ml of solvent)

Crystalline WSP solution in DMSO spin coated on PEDOT: PSS film. Micron size crystals were found all over the surface of PEDOT: PSS film.

For DI water as solvent, **Left**: (a) WSP on PEDOT: PSS - broken or pilled out films of PEDOT: PSS were found re-deposited randomly on WSP film; **Right**: (b) WSP on ITO coated glass – crystals were found on the surface and were quite loosely attached to ITO that DekTak measurement was not possible.
Substrate coating with WSP continued..

Optical images of WSP spin coated on PEDOT: PSS film when; Left: WSP solution in ethanol; Right: WSP solution in methanol. In both the cases micron size crystals were found on whole substrate.

- Solution and the substrate were heated prior to and during the spin coating using IR lamp.
- IR heating helps evaporate the solvent faster and crystal formation inhibited.

WSP solution in ethanol spin coated on a PEDOT: PSS film while substrate and solution were heated with IR lamp.  Left: WSP film in the middle of the substrate and Right: Image near the corner showing WSP film and crystals separated by a boundary.
Main fabrication steps:

ITO/PEDOT:PSS (80nm)/WSP (55nm)/C\textsubscript{60} (50nm)/Al (110nm)

Fabrication steps for WSP based OPV. The actual fabricated device is in center.
- **Fabrication steps**

  - Dicing and first cleaning (sonication in soap for 10m)
  - ITO etch (37% HCL for 6m)
  - Substrate clean (acetone 10m, IPA 5m, DI overflow rinse 3m)
  - Substrate bake and plasma clean (150C for 1 hour; 1min)
  - Spin coat PEDOT: PSS and baked (4000 rpm 1m; 120C for 15m)
  - Substrate transferred to glove box.
  - A solution of 10mg of WSP in 1ml of ethanol was prepared and filtered
  - WSP spin coated while solution and substrate heated with IR lamp (2000 rpm 1m) and baked (100C for 2m)
  - C<sub>60</sub> (49nm) thermally evaporated at a base pressure of 7x10<sup>-7</sup>torr
  - Aluminum (110nm) thermally evaporated at a base pressure of 5x10<sup>-7</sup> torr using a shadow mask
Electrical testing and discussion

- Keithley 2410 and 4155A HP Parameter Analyzer used for I-V measurements with the help of LabVIEW program.
- Calibrated Dolan-Jener Fiber Lite incandescent halogen light as input source (32mW/cm² sunlight equivalent)

J-V curve for WSP based OPV cell. 

- $V_{OC} = 0.525V$, $I_{SC} = 0.202mA/cm^2$, $FF = 0.432$, $PCE = 0.144\%$
Discussion continued..

- WSP crystallization was inhibited by using the new method to form a thin film.
- Bilayer OPV cell using WSP cells successfully fabricated and characterized.
- Fill factor and open circuit voltage for WSP based device is comparable to other pentacene based cells in literatures.
Bilayer OPV using TTPO (a new pentacene)

- 5,6,7-trithiapentacene-13-one (TTPO) synthesized by Prof. Glen Miller’s group at UNH, Durham
- It acts as a donor. High thermal stability up to 400°C
- A good film from thermal evaporation
- Increasing mobility up to 150°C observed by Erfan
- Fabricated OPV cell successfully and characterized

Chemical structure of 5,6,7-(trithia)pentacene-13-one (TTPO)
Fabrication steps

ITO/PEDOT:PSS (80nm)/TTPO (55nm)/C$_{60}$ (25nm)/Al (110nm)

- Dicing and first cleaning (sonication in soap for 10m)
- ITO etch (37% HCL for 6m)
- Substrate clean (acetone 10m, IPA 5m, DI dump-rinse 3m)
- Substrate bake and plasma clean (150C for 1 hour; 1min)
- Spin coat PEDOT: PSS and baked (4000 rpm 1m; 120C for 15m)
- 25mg of TTPO loaded in thermal evaporator at the base pressure of $5 \times 10^{-6}$ torr and evaporated to get 20nm thick TTPO
- C$_{60}$ (25nm) thermally evaporated at a base pressure of $5 \times 10^{-7}$torr
- Aluminum (110nm) thermally evaporated at a base pressure of $1.2 \times 10^{-6}$torr using a shadow mask
Electrical testing and discussion

Performance of TTPO based cells under light only and light with IR heating

<table>
<thead>
<tr>
<th>Light illumination only (Room temperature)</th>
<th>Illumination + IR heating (~80°C)</th>
<th>Illumination + IR heating (~130°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_{OC}$ (V)</td>
<td>$J_{SC}$ (mA/cm$^2$)</td>
<td>FF</td>
</tr>
<tr>
<td>0.30</td>
<td>1.50</td>
<td>0.20</td>
</tr>
<tr>
<td>0.19</td>
<td>0.14</td>
<td>0.18</td>
</tr>
<tr>
<td>0.45</td>
<td>7.78</td>
<td>0.12</td>
</tr>
<tr>
<td>0.25</td>
<td>0.015</td>
<td>0.23</td>
</tr>
</tbody>
</table>

- Best performing cell showed an efficiency of 1.5x10$^{-3}$% at 130°C. However, other cells performed better at 80°C than 130°C. Its low efficiency is possibly because of very low mobility (10$^{-9}$cm$^2$/V-s) measured by Erfan Kheirkhahi.

- At higher temp (130°C) either material degrades or chemical reactions take place.

- Increased photocurrent at raised temperatures possibly because increase in mobilities in TTPO at higher temperatures.

- Hopping transport improves in disorder systems. Mobility is proportional to $e^{(-\Delta/kT)}$, where $\Delta$ is the activation energy relating the amount of disorder. Or, localized trap states thermally activated into band states where, $k_B T >$ trap energy.
BHJ OPV using BC$_{60}$DTP (a new pentacene)

Cell structure: ITO/PEDOT:PSS(80nm)/P3HT:BC$_{60}$DTP(90-140nm)/Al(110nm)

- Bis-C$_{60}$ adduct of 6,13-(decylthio)pentacene (BC$_{60}$DTP) synthesized by Prof. Glen Miller’s group at UNH, Durham.
- Acts as an acceptor and is very stable
- Well soluble in organic solvents such as chlorobenzene
- A good film from spin coating obtained
- Fabricated OPV cell characterized
UV-Vis spectra of $\text{BC}_{60}\text{DTP}$ and $\text{C}_{60}$ in o-DCB

<table>
<thead>
<tr>
<th>Materials</th>
<th>$\text{C}_{60}$</th>
<th>$\text{BC}_{60}\text{DTP}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>LUMO (eV)</td>
<td>-3.74</td>
<td>-3.74</td>
</tr>
<tr>
<td>HOMO (eV)</td>
<td>-5.66</td>
<td>-5.44 to -5.64</td>
</tr>
<tr>
<td>Optical Bandgap (eV)</td>
<td>1.92</td>
<td>1.7 – 1.9</td>
</tr>
</tbody>
</table>

Prof. Glen Miller group’s unpublished result
Fabrication steps

ITO/PEDOT:PSS (80nm)/P3HT: BC$_{60}$DTP (65 to 140nm)/Al (110nm)
Characterization and discussion

- Tested under calibrated halogen lamp (32mW/cm² sunlight equivalent)

J-V curve for BC₆₀DTP based OPV cell

$J_{sc} = 0.417\ mA/cm²$, $V_{oc} = 0.4\ V$, $FF = 0.222$, $P_{in} = 32mW/cm²$, Efficiency = 0.116%
## Characterization and discussion

Fabrication parameters and electrical output results of OPV cell with blend of \( \text{P3HT: BC}_{60}\text{DTP (1:1 wt. ratio)} \)

<table>
<thead>
<tr>
<th>Sample #</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Active layer thickness (nm)</td>
<td>65</td>
<td>85</td>
<td>140</td>
<td>130</td>
<td>115</td>
<td>120</td>
</tr>
<tr>
<td>Post spin-coat baking (°C, min)</td>
<td>120°C, 2m</td>
<td>120°C, 2m</td>
<td>120°C, 2m</td>
<td>120°C, 2m</td>
<td>No bake</td>
<td>No bake</td>
</tr>
<tr>
<td>Post fabrication bake (°C, min)</td>
<td>100°C, 1m</td>
<td>100°C, 1m</td>
<td>100°C, 1m</td>
<td>100°C, 1m</td>
<td>100°C, 1m</td>
<td>100°C, 1m</td>
</tr>
<tr>
<td>( J_{sc} ) (µA/cm²)</td>
<td>120</td>
<td>162</td>
<td>356</td>
<td>417</td>
<td>1.7</td>
<td>2</td>
</tr>
<tr>
<td>( V_{oc} ) (V)</td>
<td>0.50</td>
<td>0.47</td>
<td>0.24</td>
<td>0.40</td>
<td>0.10</td>
<td>0.31</td>
</tr>
<tr>
<td>FF</td>
<td>0.18</td>
<td>0.23</td>
<td>0.19</td>
<td>0.222</td>
<td>0.19</td>
<td>0.12</td>
</tr>
<tr>
<td>% PCE</td>
<td>0.034</td>
<td>0.055</td>
<td>0.05</td>
<td>0.115</td>
<td>1×10⁻⁴</td>
<td>2×10⁻⁴</td>
</tr>
</tbody>
</table>

Thicker active layers (130nm and 140nm) showed higher short circuit currents. Cells with 115nm and 120nm thick layers show very poor performance.
Discussion

- The cell showed maximum efficiency of 0.116% only.

- A very low hole mobility could be one reason for such low fill factor and low short circuit current.

- Without post spin-coat baking, cells almost does not show a short circuit current due to possible chemical degradation of BC$_{60}$DTP in the solvent for long hours.
Device model for bilayer organic solar cell

Exciton model

Active bilayers of OPV cell. Light falls at $x=0$. Donor-acceptor (D-A) interface is at $x=d_1$. Donor and acceptor thicknesses are $d_1$ and $d_2$, resp. $J_{ex,1}$ and $J_{ex,2}$ are exciton flux densities at the interface.

Exciton diffusion: $D_{ex} \frac{d^2 n_{ex}}{dx^2} + \alpha \phi_0 e^{-\alpha x} - \frac{n_{ex}}{\tau_0} = 0$

Exciton flux densities at interface:

$$J_{ex,1} = \frac{\alpha_1 \phi_0 e^{-\alpha_1 d_1}}{(\beta_1^2 - \alpha_1^2)} \left[ \alpha_1 - \beta_1 + 2\beta_1 + \frac{e^{\beta_1 d_1} - e^{-\beta_1 d_1}}{e^{\beta_1 d_1} - e^{-\beta_1 d_1}} \right]$$

$$J_{ex,2} = \frac{-\alpha_2 \phi_0 e^{-\alpha_2 d_1}}{(\beta_2^2 - \alpha_2^2)} \left[ \alpha_2 - \beta_2 - 2\beta_2 + \frac{e^{-\beta_2 d_2} - e^{-\alpha_2 d_2}}{e^{-\beta_2 d_2} - e^{-\alpha_2 d_2}} \right]$$

Exciton flux density at interface: $J_{ex,i} = J_{ex,1} + J_{ex,2}$

Total exciton flux density: $J_G = \int J_{ex,i} (\alpha(\lambda), \phi_0(\lambda)) d\lambda$

Carrier transport model

Poisson equation:
\[
\frac{d^2\psi}{dx^2} = \frac{q}{\varepsilon} [n_e - n_h]
\]

Drift-diffusion equations:
\[
J_{e(h)} = q \left[ n_{e(h)} \mu_{e(h)} E \pm D_{e(h)} \frac{dn_{e(h)}}{dx} \right]
\]

Recombination equation:
\[
R = \gamma \left[ n_e n_h - n_{int}^2 \right]
\gamma = \frac{q}{\varepsilon} (\mu_e + \mu_h)
\]
\[
\frac{dJ_{e(h)}}{dx} = \mp q \left( \frac{J_{ex,i}}{W_{int}} - R_{e(h)} \right)
\]

Boundary conditions:
\[
n_e \mid_{x=d} = N_c e^{-\frac{\Phi_c-LUMO}{kT}}
\]
\[
n_h \mid_{x=0} = N_v e^{-\frac{HOMO_D-\Phi_a}{kT}}
\]

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>(d_1, d_2)</td>
<td>Thickness of front and back layer</td>
<td>10 to 90nm</td>
</tr>
<tr>
<td>(\mu_e, \mu_h)</td>
<td>Mobility of electron in acceptor and hole in donor</td>
<td>(10^{-7}) to (10^{-3}) cm(^2)/V.s</td>
</tr>
<tr>
<td>(W_{int})</td>
<td>Effective width of the D-A interface</td>
<td>0.8nm</td>
</tr>
<tr>
<td>(L_{Dex})</td>
<td>Exciton diffusion lengths in donor and acceptor</td>
<td>20nm, 5nm</td>
</tr>
<tr>
<td>(N_c, N_v)</td>
<td>Effective density of states</td>
<td>(10^{21}) /cm(^3)</td>
</tr>
<tr>
<td>(\varepsilon_r)</td>
<td>Relative permittivity</td>
<td>3</td>
</tr>
<tr>
<td>(n_{int})</td>
<td>Intrinsic carrier density at D-A interface</td>
<td>(10^{11}) /cm(^3)</td>
</tr>
<tr>
<td>(\gamma)</td>
<td>Langevin bimolecular recombination strength</td>
<td>/cm(^3)/s</td>
</tr>
<tr>
<td>(D_e, D_h)</td>
<td>Diffusion coefficients of electron and holes, respectively</td>
<td>(k_B T \mu_{e(h)}/q)</td>
</tr>
<tr>
<td>(LUMO_{D(A)})</td>
<td>Lowest unoccupied molecular orbital of donor and acceptor</td>
<td>3.0 eV, 3.7 eV</td>
</tr>
<tr>
<td>(HOMO_{D(A)})</td>
<td>Highest occupied molecular orbital of donor and acceptor</td>
<td>4.9 eV, 6.0 eV</td>
</tr>
<tr>
<td>(\Phi_c, \Phi_a)</td>
<td>Cathode &amp; anode work functions</td>
<td>3.9 eV, 4.7 eV</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\phi_{ex})</td>
<td>Wavelength dependent photon flux density</td>
<td>/cm(^2)/s</td>
</tr>
<tr>
<td>(\alpha)</td>
<td>Wavelength dependent absorption coefficient</td>
<td>/cm</td>
</tr>
<tr>
<td>(n_{ex})</td>
<td>Steady state exciton density</td>
<td>/cm(^3)</td>
</tr>
<tr>
<td>(J_{e(h)})</td>
<td>Electron (hole) current density in acceptor (donor)</td>
<td>mA/cm(^2)</td>
</tr>
</tbody>
</table>
J-V characteristics of simulated bilayer OPV cell. Thickness $d_1 = d_2 = 50$nm; $\mu_h = \mu_e = \mu$. With increase in mobility, open circuit voltage decreases. Short circuit current does not change much for mobility range of $10^{-5}$ - $10^{-2}$ cm$^2$/V-s but decreases with decrease in mobility below $10^{-5}$ cm$^2$/V-s.

OPV power conversion efficiency at various mobilities ($\mu_h = \mu_e = 10^{-7}$ to $10^{-2}$ cm$^2$/V-s) for donor and acceptor thicknesses of 50nm each. PCE increases with mobility increase until it reaches to maximum at mobility = $10^{-4}$ cm$^2$/V-s. PCE starts decreasing thereafter.
Relative levels of HOMO-LUMO energy of donor and acceptor in open circuit condition for three mobilities ($\mu_h=\mu_e=\mu$) $10^{-6}$ cm$^2$/V-s, $10^{-4}$ cm$^2$/V-s and $10^{-2}$ cm$^2$/V-s. Donor LUMO level is set at 0 eV for the convenience. The thickness of the donor and the acceptor both are 50 nm and D-A interface is at distance 0. As mobility increases, the difference between the donor LUMO and the acceptor LUMO increases and thus, the split between the donor HOMO and the acceptor LUMO decreases.
Power conversion efficiency of OPV device with donor thicknesses [10, 30, 50, 70, 90] nm, acceptor thickness 50nm and mobilities $\mu_h = \mu_e = [10^{-6}, 10^{-5}, 10^{-4}, 10^{-3}, 10^{-2}] \text{ cm}^2/\text{V-s}$. PCE is found to be maximum of 0.67% at 50nm thick donor with electron and hole mobility of $10^{-4} \text{ cm}^2/\text{V-s}$. Simulation results continued …
Power conversion efficiency of OPV for acceptor thicknesses [10, 30, 50] nm, donor thicknesses [10, 30, 50, 70, 90] nm, and mobilities $\mu_h = \mu_e = \mu = [10^{-6}, 10^{-5}, 10^{-4}, 10^{-3}, 10^{-2}]$ cm$^2$/V-s. For mobility range $\mu = [10^{-6}-10^{-5}]$ cm$^2$/V-s, maximum PCE is found to be 0.59 % when the donor thickness is 30nm and the acceptor thickness is 10nm (dashed line surface). For higher mobility range $\mu = [10^{-4}- 10^{-2}]$ cm$^2$/V-s, maximum PCE is found to be 0.67 % for 50nm thick donor and 50nm thick acceptor (solid line surface).
Percentage power conversion efficiency (PCE) of OPV device for electrons and holes mobilities both varying from $[10^{-7} \text{ to } 10^{-2}] \text{ cm}^2/\text{V-s}$. Maximum PCE of 0.67% is found at electrons and holes mobilities, $\mu_h = \mu_e = 10^{-4}\text{cm}^2/\text{V-s}$. Further increases in mobilities, the conversion efficiency slightly decreases.
Simulation results continued …

Bar plot of percentage change in PCE for various mobilities and mobility imbalance ratios. For higher mobilities ($10^{-4}$, $10^{-3}$) cm$^2$/V-s, PCE drops at even lower mobility ratio ($10^1$). For lower mobilities ($10^{-6}$, $10^{-7}$) cm$^2$/V-s, PCE drops at higher mobility ratios ($>10^4$).
Conclusions

- WSP crystallization was inhibited by using the new method to form a thin film. Fabricated bilayer OPV cell using WSP cells has fill factor and open circuit voltage comparable to other pentacene based cells in literatures. But the overall efficiency is quite low 0.145%.

- TTPO based cell showed maximum efficiency of 1.5x10^{-3}%. It is found to be showing increased photocurrent at raised temperatures but performance goes down above 80°C. Its very low mobility (~10^{-9} cm²/V-s) could be possible cause for such low efficiency.

- BC_{60}DTP based bulk heterojunction cell showed maximum efficiency of 0.116%. Without post spin-coat baking, cells almost do not show a short circuit current due to possible chemical degradation of BC_{60}DTP in the solvent. A very low hole mobility could be one reason for cell’s low fill factor and low short circuit current.

- With our improved model, OPV devices are simulated and optimal thicknesses of donor and acceptor both were found to be 50nm. For maximum PCE, the optimal mobility was found to be about 10^{-4} cm²/V-s and about 15% decrease is observed for high mobility (10^{-2} cm²/V-s). Pure imbalance in mobilities does not degrade PCE.
Future Work and Suggestions

• Mobility extraction of WSP and BC_{60}DTP.

• Thickness optimization of active layers of WSP and BC_{60}DTP based cells.

• Use of three dimensional substrate by assembly of ITO nanoparticles on ITO plane surface to form nanopillars.

• Use of neutral PEDOT: PSS or MoO_{3} as electron blocking layer in WSP based cells.

• Use of TiO_{2} nanoparticles as acceptor to fabricate a WSP based bulk heterojunction solar cell.

• A blend of P3HT: BC_{60}DTP in a ratio of 2:1 may be a better matching of donor-acceptor interface for more efficient charge dissociation

• Coat OPV cells with parylene and evaluate the time dependent performance.
Thank You

Questions ?
Electron and hole blocking layers for WSP

Electron blocking layer

- PEDOT: PSS solution is acidic whereas WSP a basic
- Use of 2-dimethylaminoethanol (DMAE) to neutralize the PEDOT: PSS solution (Appl. Phys. Lett., 2010. 96(15))
- ITO nanopillars
  - ITO nanopillars based OPV cell (not reported)
  - ZnO nanorodes in DSSC and OPV reported in several literatures to increase the interface area
  - To increase the percolated path in bulk heterojunction
Parylene encapsulation

Encapsulation

- Inexpensive
- High tensile and yield strength
- Conformal and tension free coating
- Excellent transparency in visible light and UV light absorber
- Outstanding barrier to moisture and gases
- Intend to coat parylene on OPV cell and compare the time dependent performance (Synthetic Metals, 2005. 155(2))
Concentration (/cm$^3$) of holes in the donor and electrons in the acceptor for various mobilities ($\mu_h = \mu_e = \mu$). The thickness of the donor and the acceptor both are 50nm and D-A interface is at distance 0. The charge accumulation at the D-A interface decreases with increasing mobility.

Electric field in the donor and the acceptor for various mobilities ($\mu_h = \mu_e = \mu$) in open circuit condition. The thickness of the donor and the acceptor both are 50nm and D-A interface is at distance 0. Electric field at D-A interface increases with increasing mobility.