Introduction to Organic Solar Cells

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Organic semiconductors

- Conductivity in polyacetylene – 1970s – Nobel Prize

  Alan J. Heeger  Alan G. MacDiarmid  Hideki Shirakawa

- Interacting $P_z$ orbitals create chain of delocalised electron density

poly(phenylene vinylene) (PPV)
Why organic materials for solar cells?

- Room temperature
- Ambient pressure
- Solution-processing
Research activity in organic PV

- ISI - all databases
  - “Organic photovoltaics”
  - “Organic solar cells”
  - “Plastic photovoltaics”
  - “Plastic solar cells”
CSIRO organic PV – since 2005

- Division of Energy Technology
  - National Solar Energy Centre – Newcastle
  - Axial device design (cell structures)
  - Lateral device design (modules)

- Division of Molecular and Health Technologies – Melbourne
  - Long record of achievements in materials chemistry
Measuring efficiency to IEC60904
The single semiconductor device

Metal back contact (cathode)

Exciton (bound)

Transparent front contact (anode)

c-Si (300μm)

organic solar cell (100nm)

Al/Ca

organic semiconductor ~100nm

ITO/PEDOT:PSS

Transparent front contact (anode)

Al/Ca

Metal back contact (cathode)

Cathode

Anode

ITO/PEDOT:PSS

c-Si (300μm)

organic solar cell (100nm)
Splitting excitons: The planar heterojunction

anode          donor          acceptor          cathode

poly (3-hexylthiophene) - P3HT  [6,6]-phenyl-C61 butyric acid methyl ester - PCBM

HOMO       LUMO

LUMO       HOMO

Energy / eV

P3HT Total DOS

0  -1  -2  -3  -4  -5  -6  -7  -8  -9
20   15   10   5   0
Total DOS

PCBM Total DOS

0  -1  -2  -3  -4  -5  -6  -7  -8  -9
0   2   4   6   8   10  12  14
Total DOS

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Understanding open-circuit voltage

- Heterojunction – voltage can go beyond flat-band

1. Bands prior to assembly

2. Assembled device (planar heterojunction)

3. Illuminated to flat-band voltage

4. Illuminated beyond flat-band voltage
The bulk heterojunction device

- Mix donor and acceptor into one blend
- Greatly increases interface area for exciton dissociation
- Nanomorphology now critical
  - Choice of solvent
  - Annealing
- Penalties in voltage and transport
1: Exciton generation

2: Exciton dissociation

3: Charge transport

Understanding photocurrent
1: Exciton generation (optical excitation)

• How much light is coupled into the active layer?
  • Measure the optical properties of each layer, \( n(\lambda) \) and \( k(\lambda) \)
  • Use Fresnel equations to model multi-layer interference
Photon accounting

Active Layer 1:1 Wavelength Distribution 38nm
Active Layer 1:1 Wavelength Distribution 81nm
Active Layer 1:1 Wavelength Distribution 252nm

ENERGY

EXCITONS

38nm active layer
81nm active layer
252nm active layer

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Internal quantum efficiency

Calculation: IQE decreases with thickness of active layer.

Measurement: Short-circuit current density and cell voltage vary with active layer thickness.

IQE decreases with thickness of active layer.
2: Exciton dissociation

- Two-stage process
  - Rapid dissociation to polaron pair
  - Polaron pair separation efficiency – FIELD DEPENDENT

- Photocurrent is voltage-dependent!
3: Charge transport - hopping

- Space charge contribution to the electric field

\[
\frac{dE(x)}{dx} = \frac{e}{\varepsilon \varepsilon_0} [p(x) - n(x)]
\]

- Transport equation for electrons

\[
J_e(x) = e \mu_e (E, T) n(x) E(x) + D(\mu, T) \frac{dn(x)}{dx}
\]

- Continuity equation for electrons

\[
\frac{dn(x)}{dt} = \frac{1}{e} \frac{dJ_e(x)}{dx} + k_d S(x) - R(x)
\]
Bi-molecular recombination

- Hopping transport
  - Band-band (intrinsic) recombination rate not important

- Bi-molecular recombination rate dominated by the time it takes for carriers to meet

- Langevin-type recombination

\[ R(x) = \frac{q}{\varepsilon \varepsilon_0} \min\{\mu_e, \mu_h\} n(x)p(x) \]

- Higher mobility means greater recombination!
Opportunities to increase performance

• Improving absorption
  • Narrow spectral bandwidth limits capture of AM1.5

• Optimise band structure
  • Adjusting heterojunction band offsets to minimise energy loss whilst still splitting exciton

• Improving mobility
  • Higher mobility materials
  • Interdigitated donor-acceptor designs for simpler carrier pathways

• Optimising optical interference
  • Maximise light-trapping in the active layer

• Reducing exciton binding energy
  • The biggest single obstacle to reaching the Shockley-Queisser limit
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Thank you