Nanostructured and molecular materials for solar energy conversion

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Printable photovoltaics

- Variety of materials
- Process from solution
- “One pot, one shot” active layer

- Large area
- High throughput
- Printing or coating

- Conformal
- Lightweight
- Cheap
Why print photovoltaics?

- Minimise production costs
- New product forms
- Potential for innovation in manufacturing
- Reduce carbon embedded in manufacture
Solution processable photovoltaic materials

1990- Dye sensitised

\[ \eta \approx 12\% \]

1990: Dye sensitised

2001- Organic (polymer:C60)

\[ \eta \approx 10\% \]

2001: Organic (polymer:C60)

2007- Organic tandem

\[ \eta \approx 11\% \]

2007: Organic tandem

2010- Particle slurry CZTS

\[ \eta \approx 12\% \]

2010: Particle slurry CZTS

2012- Perovskite

\[ \eta \approx 16\% \]

2012: Perovskite

Other new materials and new processes...
Molecular electronic materials

- Electronic properties:
  - Excited states and charged states are **localised**
  - Electronic states are **disordered**
  - Low relative permittivity $\varepsilon_r$

- Charge transport is slow
- Charge pairs hard to separate
Photovoltaic energy conversion in molecular materials

Separate charges by adding a strong electron acceptor

Distributed heterojunction $\Leftrightarrow$ charge separation over a large optical depth

Photocurrent direction provided by asymmetric contacts

Photovoltage limited by electrical gap $E_{CS}$ (< optical gap $E_g$)
Materials development

![Graph showing efficiency (%) over years from 2000 to 2015.]

- **2001**: 2.5% (Schaarber et al., Adv. Mater. 2006)
- **2005**: 4.4%
- **2007**: 5.5%
- **2009**: 6% (9.2% in 2011)

Theoretical limit?

![Chemical structures and theoretical limits for HOMO and LUMO levels.]

**Band Gap [eV]**
- 2.8
- 2.4
- 2.0
- 1.6
- 1.2
- 0
- -3.2
- -3.4
- -3.6
- -4.0

**LUMO Level Donor [eV]**
- 1.0
- 9.0
- 10.0
- 11.0

**Reducing gap & increasing E_{CS}**

**Increasing E_{CS}**

**Decreasing optical gap**

**ΔE_c**

**E_{CS}**

**E_g**

**E_{Voc}**

**HOMO**

**LUMO**

**donor**

**acceptor**
Sources of loss in organic photovoltaic heterojunctions

How much do we pay for charge separation?

How much do we pay for charge recombination?
Probing charge separation

- Probe the energy of intermediate state using electroluminescence

- Probe the yield of charge pairs using transient spectroscopy
Probing charge separation

- Influenced by
  - Specific chemical structure and alignment
  - Molecular packing close to interface
  - Competition with other excited states

Normally > 0.3 eV

Limiting efficiency < 20%
Sources of loss in organic photovoltaic heterojunctions

How much do we pay for charge separation?

How much do we pay for charge recombination?
Nature of charge recombination

- Electronic state energies are disordered
- Recombination occurs between free and trapped charges
- Density dependent mobility and lifetime
- Intensity dependent PV performance

\[
\frac{1}{e} \nabla \cdot \mathbf{J} = G - R
\]
Example: Effect of fullerene structure on charge collection

Fullerene multi-adducts

Reduce photocurrent

Why?

Energetic disorder?

Packing disorder?

Example: Modelling effect of fullerene structure

Coarse grain

Representative structures

Electronic coupling & transport

Distinguish effects

F. Steiner, J. M. Frost et al (2014)
Where do we go from here?

- Solar electricity is abundant, sustainable, versatile and available
- To accelerate its use, cheaper materials or technologies are needed
- Nanostructured and molecular materials offer potential for radically different and cheaper solar-electric conversion technologies.
- Challenges remain for physicists, chemists and materials scientists – but none of them known to be insurmountable
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