Engineering new molecules for photovoltaic applications

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Solar energy harvesting
Solar energy harvesting

Cao, Gamelin, Ginger, Hillhouse, Jen, Jenekhe, Luscombe
US solar resources and the myth

Installed 0.9 GWp (<0.01%) of Capacity in 2010

Installed 7.2 GWp (3%) of Capacity in 2010
Photovoltaic efficiencies

Best Research-Cell Efficiencies

- **Multijunction Cells** (2-terminal, monolithic)
  - Three-junction (concentrator)
  - Three-junction (non-concentrator)
  - Two-junction (concentrator)
- **Single-Junction GaAs**
  - Single crystal
  - Concentrator
  - Thin film crystal
- **Crystalline Si Cells**
  - Single crystal
  - Multicrystalline
  - Thick Si film
  - Silicon Heterostructures (HIT)
- **Thin-Film Technologies**
  - Cu(In,Ga)Se_2
  - CdTe
  - Amonorphous Si/II/ (stabilized)
  - Nano- micro- poly-Si
  - Multijunction polycrystalline
- **Emerging PV**
  - Dye-sensitized cells
  - Organic cells (various types)
  - Organic tandem cells
  - Inorganic cells
  - Quantum dot cells

Research organizations and laboratories involved:
- IBM (T. J. Watson Research Center)
- Varian
- Stanford (140x)
- Japan Energy
- NREL Spectrolab
- Spectrolab (4.0% - 14nm)
- ISU (10%)
- Sharp (15x)
- First Solar
- LG Electronics
- Mitsubishi Chemical
- SunPower
- Fraunhofer ISE
- NREL (Inverted metamorphic)
- Sharp (17%)
- Solar Junction (all devices)

Innovations and milestones:
- 1975: First solar cell demonstration
- 2015: Continued advancements in efficiency and technology
Solution-processible devices

Nanocrystals or Molecular Precursors or Polymers

Formulation → Ink → Bottom Contact Glass Substrate

Heat and/or Vapor Treat

Top Contact
n-type
absorber (p-type)
Bottom Contact
Glass Substrate

photoabsorbing semiconductor
Bottom Contact
Glass Substrate

Ginger, Hillhouse, Jen, Jenekhe, Luscombe

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Energy pay back time

Time needed to operate the device to recover the energy used - and also the associated generation of pollution and $\text{CO}_2$ - to make the devices in the first place.

<table>
<thead>
<tr>
<th>Material</th>
<th>10% CIGS</th>
<th>20% CIGS</th>
<th>4% OPV</th>
<th>8% OPV</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crystalline silicon</td>
<td>EPBT 2.7 yrs</td>
<td>EPBT 1 yr</td>
<td>EPBT 1/2 yr</td>
<td></td>
</tr>
</tbody>
</table>

Time needed to reach generation capacity

Using 100% of the energy generated to manufacture more cells:

- 20% CIGS
- 10% CIGS
- 8% OPV

EPBT: 2.7 yrs

Using only 50% of the energy generated to manufacture more cells:

- 16% CIGS
- 13% CIGS
- 4% OPV

EPBT: 1/2 yr

EPBT 1 yr
EPBT 2.7 yrs

Crystalline silicon

US consumes 3,300 GW (3,300,000,000 W)

Target 1,000 GW (30%)

From Hugh Hillhouse
The photovoltaic effect

Sunlight

Cathode
Acceptors
Junction
Donor
Anode

Energy levels

Donor

Acceptor
The photovoltaic effect

Sunlight

Cathode
Acceptors
Junction
Donor
Anode

Energy levels

Donor
Acceptor
The photovoltaic effect

Sunlight

Cathode

Accepter

Junction

Donor

Anode

Energy levels

1

Donor

Acceptor
The photovoltaic effect

Sunlight

Cathode

Acceptor

Junction

Donor

Anode

Energy levels

Donor

Acceptor
Design criteria for materials

- Good absorption in the visible region
- Energy levels of the n and p-type semiconductors must match well
- Good interaction between the two materials
- High charge mobility
- Solution processible
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Low band gap polymers

Macromolecules, 2012, 45, 5934

Mingjian Yuan, Matt Durban, Peter Kazarinoff, Andrew Rice, Pinyi Yang, Katherine Mazzio; Jen, Jenekhe
Low band gap polymers

Donor

-3.63 eV

-5.3 eV

Acceptor

-3.71 eV

-4.2 eV

-6.5 eV

Macromolecules, 2012, 45, 5934

Mingjian Yuan, Matt Durban, Peter Kazarinoff, Andrew Rice, Pinyi Yang, Katherine Mazzio; Jen, Jenekhe
Low band gap polymers

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Exciton diffusion bottleneck

100 nm
Electron donor
Electron acceptor

10 nm

Microstructure of the active layer

Power Conversion Efficiencies at AM 1.5 G
Solar Intensity
PCBM:P3HT 1:1 Thin film from chlorobenzene
Annealed at 140 °C

PCBM:P3HT 1:1 Thin film from chlorobenzene
TOP: no anneal BOTTOM: 140 °C 1 h
Low band gap polymers

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Step growth polymerization

• Broad molecular weights

• Molecular weight is heavily dependent on the purity of the monomer (a decrease in purity by 0.1% can decrease molecular weight by up to 50%)

• Leads to batch-to-batch variability

• Optoelectronic properties vary which means fluctuating electronic device performance
Chain growth polymerization

- One monomer at a time adds to the growing polymer chain.
- Under certain conditions, the polymerization can be controlled to produce specific molecular weights with narrow polydispersities (living polymerization)
Alternate polymer architectures

**Star-shaped polymers**

**Block copolymers**

A living polymerization would give us the ability to dial in specific monomers and shapes into the polymer, and provide us with a better handle to control properties and morphology in a reproducible manner.
Quasi-living polymerization of 3HT

Quasi-living polymerization of 3HT

Shane Boyd, Hugo Bronstein, Natasha Doubina, Ken Okamoto, Prakash Sista, Mingjian Yuan
Alternate polymer architectures

Star-shaped polymer

Surface-initiated polymerization

Hugo Bronstein, Natasha Doubina, Ken Okamoto, Prakash Sista, Mingjian Yuan
NSF SEP: Sustainable Pathway to Terawatt-Scale

Solution-processed solar cells from earth abundant elements

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