Center for Advanced Molecular Photovoltaics

Director: Mike McGehee
Executive Director: Alan Sellinger
Deputy Director: Peter Peumans

$5 million/year for five years from Saudi Arabia (KAUST)
Background on KAUST

• King Abdullah University of Science & Technology (KAUST)
  http://www.kaust.edu.sa/
  – Endowment of $20 B
  – Women and men educated together.
  – Research thrusts in:
    • Resources, Energy and Environment
    • Biosciences and Bioengineering
    • Materials Science and Engineering
    • Applied Mathematics and Computational Science
KAUST in May 2008
KAUST one month later
KAUST future (opening Sep. 2009)
Covering less than 1 % of the land with solar cells could meet our electricity needs

6 Boxes at 3.3 TW Each
Large Scale Printing of Semiconductors!
Molecular Semiconductors

Attractive properties:

• Abundant: ~100,000 tons/year
• Mature industry/markets
• Low materials cost: ~1$/g → 17¢/m²
• Low-cost manufacturing
• Non-toxic

CuPc
Copper Phthalocyanine
OPV Efficiency Status: Lab-Cells

Best Research-Cell Efficiencies

Source L.L. Kazmerski, NREL
## CAMP Goals

<table>
<thead>
<tr>
<th>Molecular PV</th>
<th>Silicon PV</th>
</tr>
</thead>
<tbody>
<tr>
<td>• 15% Efficiency</td>
<td>• 12% Efficiency</td>
</tr>
<tr>
<td>• 10-20 year lifetime</td>
<td>• &gt;20 year lifetime</td>
</tr>
<tr>
<td>• $30/m²</td>
<td>• $350/m²</td>
</tr>
</tbody>
</table>

Training of top quality students for solar industry!
Power Conversion Efficiency (PCE)

\[ \eta = \frac{FF \times Isc \times V_{OC}}{\text{Incident Power}} \]

Physics of Organic Solar Cells

Forrest, MRS Bulletin 2005
Device Fabrication and Characterization

Mike McGehee

Peter Peumans

Michael Graetzel (EPFL)
Polymer-fullerene bulk heterojunction cells

PEDOT

Ca/Al

~200 nm thick
X-ray Diffraction pBTTT:PC$_{[71]}$BM Blends

- 1:0
- (400)$_p$, (300)$_p$, (200)$_p$, (100)$_p$, (003)$_p$
- (010)$_p$

- 1:1
- (500)$_i$, (402)$_i$
- (400)$_i$, (300)$_i$, (200)$_i$, (001)$_i$, (010)$_i$, (020)$_i$

- 1:4
- PC$_{[71]}$BM

Structural diagrams:

- ~21.5 Å
- 30 Å
Consequences of Intercalation

Dense Side-Chains

- e.g. P3HT
- Optimal blend ratio $\sim 1:1$
- Better for avoiding back electron transfer

Less Dense Side-Chains

- e.g. pBTTT
- Optimal blend ratio $\sim 1:3$
- Better for splitting excitons
Effect of Electrical Doping

Calculated Band Diagrams

Donor and acceptor are highly doped

Donor is highly doped, acceptor ~ intrinsic

Dye sensitized solar cells

Dye: Z907

HTM: Spiro-OMeTAD (Spiro)

World Record: ~5% Efficiency

Increasing absorption in dye sensitized cells with energy relay dyes

Interface characterization and modification: Stacey Bent

Brian Hardin, Eric Hoke, McGehee, Gratzel
Advanced Optics

Peter Peumans, Mark Brongersma and Shanhui Fan
Transparent Electrodes

What’s wrong with ITO?

• Performance
• Cost (~$10/m²)
• Brittle
• Compatibility with plastic substrates
Carbon Nanotube Electrodes

<table>
<thead>
<tr>
<th></th>
<th>Efficiency</th>
<th>$J_{sc}$ (mA/cm²)</th>
<th>$V_{oc}$ (mV)</th>
<th>Fill Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>CNT cell</td>
<td>2.5%</td>
<td>7.8 mA/cm²</td>
<td>605 mV</td>
<td>0.52</td>
</tr>
<tr>
<td>ITO cell</td>
<td>3.0%</td>
<td>8.0 mA/cm²</td>
<td>610 mV</td>
<td>0.61</td>
</tr>
</tbody>
</table>

M.W.Rowell, et al, APL 2006
Ag Nanowires

Ag Nanowires

~20% of transmitted light is scattered

Radius= 8.36 mm
12.5 ohm/sq

Radius= 13.74 mm
12.6 ohm/sq

Radius= 4 mm
12.7 ohm/sq

Flat
12.7 ohm/sq

Radius= 8.36 mm
12.5 ohm/sq
ZnO Nanowires

Film cast from nw solution

milky diffusing films

Alberto Salleo
Molecular Design and Synthesis
Quantum-Chemical Calculations

Jean-Luc Bredas (Georgia Tech)

Donor-Acceptor Copolymers

\[ X = \text{C(CH}_3)_2, \text{Si(CH}_3)_2, \text{NCH}_3 \]

\[ Y = \]

Vertical Transition Energies
Quantum-Chemical Calculations

Jean-Luc Bredas (Georgia Tech)
Synthesis

Zhenan Bao
Mark Thompson (USC)
Jean Fréchet (UC Berkeley)
Alan Sellinger
Types of Materials for Organic Solar Cells

• **p-type (electron donating materials)**
  – Aromatic amines, thiophenes
  – \( \approx 90\% \) of journal publications related to p-type materials

• **n-type materials (electron accepting materials)**
  – Primarily fullerene derivatives
  – Cyano aromatics, perylene diimides, benzothiadiazole
  – Area relatively unexplored due to not-so-straightforward chemistry
Sellinger Group

- Can be thermally sublimed as well

Solubilizing groups for solution processing
Conjugated chemical links
Electron accepting sites

V-BT H
Better solubility

V-BT EH
80°C device: \( V_{oc} = 0.97 \text{ V}, \) \( FF = 0.41, \) \( PCE = 1.09\% \)

80 °C device: \( V_{oc} = 1.36 \text{ V}, \) \( FF = 0.49, \) \( PCE = 0.75\% \)

Ooi, Z; Tam, TL; Shin, RYC; Chen ZK; Kietzke, T; Baumgarten, M; Mullen, K; deMello, JC; Sellinger, A, *Journal of Materials Chemistry*, 2008, 18, 4619–4622.
Work from Mark Thompson’s group at USC

Controlling $V_{oc}$

- $V_{oc}$ should correlate with the energy gap: acceptor LUMO - donor HOMO
  - $V_{oc} \propto I_g$
- Boron subphthalocyanines
  - Lower homologues of phthalocyanines
  - Nonplanar cone-shaped structure
  - Tunable HOMO and LUMO
Work from Mark Thompson’s group at USC

Energetics of Peripherally Substituted SubPcs

CuPc

C60

$E_g = 1.0\, \text{eV}$

$E_g = 1.5\, \text{eV}$

$E_g = 1.7\, \text{eV}$

$E_g = 1.9\, \text{eV}$
Work from Mark Thompson’s group at USC

Increasing $V_{oc}$

<table>
<thead>
<tr>
<th>Donor</th>
<th>$I_g$ (eV)</th>
<th>$V_{oc}$ (V)</th>
<th>FF</th>
<th>$\eta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>CuPc</td>
<td>1.5</td>
<td>0.42</td>
<td>0.58</td>
<td>0.9</td>
</tr>
<tr>
<td>SubPc</td>
<td>1.9</td>
<td>0.97</td>
<td>0.57</td>
<td>2.1</td>
</tr>
</tbody>
</table>

Work from Zhenan Bao’s group at Stanford

Bao, Z et al, manuscript in preparation
Work from Zhenan Bao’s group at Stanford

Work from Jean Fréchet’s group at UC Berkeley

Morphology Control through Regioregularity

55:45 ratio blend film
Annealed at 150°C for 3hr

RR = 86%

86%RR P3HT

Lowering RR improves the thermal stability of P3HT:PCBM BHJ devices.

Thompson, BC et al, Macromolecules 2007, 40, 7425-7428
Reliability

Reiner Dauskardt
Degradation and Reliability of Photovoltaic Devices

Severe operating environments.
Exposure to moisture, chemically active environmental species, thermal cycling and UV radiation.
Lifetimes are dictated by the loss of adhesion and defect evolution.

Characterize and model mechanisms of defect initiation and evolution accelerated by environment, thermo-mechanical cycling and UV exposure.
Adhesion/Cohesion Sample Preparation

Fabricated 4-point bend adhesion and DCB cohesion test structures using standard epoxy bonding techniques. Similar transparent glass substrates on each side.

Glass Substrate

ITO (150 nm)
PEDOT:PSS (50-100 nm)
P3HT/PCBM (200 nm)
Epoxy Bond (2 μm)
Al (100 nm)
Ca (7 nm)


Thin films sandwiched between elastic substrates

FPB adhesion

DCB cohesion
Adhesion/Cohesion Sample Preparation

- XPS reveals similar debond path for DCB and 4-pt bend samples
- C ~ 92%, S ~ 6%, O ~ 2%
- **Suggests cohesive failure in PCBM:P3HT layer and not at the interfaces!**

Conclusions

• Exciting new research activities in CAMP at Stanford University + partner universities
  – Very interdisciplinary!

• Working closely with KAUST from Saudi Arabia

• More information: Alan Sellinger (aselli@stanford.edu)