Advanced Nano materials for solar cell applications

Dhayalan Velauthapillai, HIB
World Meteorological Organization’s statement
Nov. 2014

• 2014 on track to being among hottest on record
• The global average air temperature over land and sea surface for January to October was about 0.57° Centigrade (1.03 Fahrenheit) above the average of 14.00°C (57.2 °F) for the 1961-1990 reference period
• Lima Talks - goal is to reduce greenhouse gas emissions to limit the global temperature increase to 2 degrees Celsius above current levels
Energy Use per Capita

The World Bank: Kilograms of oil equivalent (2011)
http://en.wikipedia.org/wiki/List_of_countries_by_energy_consumption_per_capita
Total Electricity Consumption vs. Electricity from Renewables

- **China**: Total Electricity Consumption = 4208 billion kilowatthours, Electricity from Renewables = 801 billion kilowatthours
- **United States**: Total Electricity Consumption = 3883 billion kilowatthours, Electricity from Renewables = 527 billion kilowatthours
- **Brazil**: Total Electricity Consumption = 479 billion kilowatthours, Electricity from Renewables = 459 billion kilowatthours
- **Canada**: Total Electricity Consumption = 552 billion kilowatthours, Electricity from Renewables = 398 billion kilowatthours
- **Russia**: Total Electricity Consumption = 869 billion kilowatthours, Electricity from Renewables = 167 billion kilowatthours
- **India**: Total Electricity Consumption = 758 billion kilowatthours, Electricity from Renewables = 160 billion kilowatthours
- **Germany**: Total Electricity Consumption = 538 billion kilowatthours, Electricity from Renewables = 126 billion kilowatthours
- **Norway**: Total Electricity Consumption = 244 billion kilowatthours, Electricity from Renewables = 111 billion kilowatthours
- **Japan**: Total Electricity Consumption = 983 billion kilowatthours, Electricity from Renewables = 116 billion kilowatthours
- **Spain**: Total Electricity Consumption = 244 billion kilowatthours, Electricity from Renewables = 87 billion kilowatthours

June 2014

Source: Energy Information Administration, International Energy Statistics
World Energy Consumption By Fuel 2012

- Natural Gas: 23.9%
- Oil: 33.1%
- Coal: 29.9%
- Nuclear Energy: 4.5%
- Hydro electric: 6.7%
- Other Energy: 1.9%

Source: The Cultural Economist
Data from BP
Adjusted World Energy Consumption By Fuel 2050

- Coal: 25.1%
- Nuclear Energy: 7.5%
- Hydroelectric: 9.2%
- Natural Gas: 25.1%
- Other Energy: 11.8%
- Oil: 21.4%

Source: The Cultural Economist
solar spectrum (terrestrial)

\[ AMX = \frac{1}{\cos \theta_x} \]

ATMOSPHERE

\( \theta_x \)

Earth

Integrated power = 100 mW/cm²

http://en.wikipedia.org/wiki/Air_mass_(solar_energy)

Gigawatts

World Total
177 Gigawatts

REN21 Renewables 2015 Global Status Report
Solar PV Capacity and Additions, Top 10 Countries, 2014

- **Germany**: +1.9 GW (2014), Total: 40.6 GW
- **China**: +10.6 GW (2014), Total: 63.3 GW
- **Japan**: +9.7 GW (2014), Total: 28.4 GW
- **Italy**: +0.4 GW (2014), Total: 10.4 GW
- **United States**: +6.2 GW (2014), Total: 35.8 GW
- **France**: +0.9 GW (2014), Total: 4.3 GW
- **Spain**: ~0 GW (2014), Total: 10.1 GW
- **United Kingdom**: +2.4 GW (2014), Total: 17.8 GW
- **Australia**: +0.9 GW (2014), Total: 6.8 GW
- **India**: +0.7 GW (2014), Total: 15.3 GW

Estimated Renewable Energy Share of Global Electricity Production, End-2014

Fossil fuels and nuclear  
77.2%

Renewable electricity  
22.8%

Hydropower  
16.6%

Wind  
3.1%

Bio-power  
1.8%

Solar PV  
0.9%

Geothermal, CSP, and ocean  
0.4%

Based on renewable generating capacity in operation at year-end 2014.

REN21 Renewables 2015 Global Status Report
how many photons can be absorbed?

Example: Silicon $E_g = 1.1 \text{eV}$. Only photons with a wavelength smaller than 1.1 $\mu$m will be absorbed.

Solar spectrum (AM1.5G)

Lundstrom, 2011
Solar Cell – Basics

The operation of a photovoltaic (PV) cell requires 3 basic attributes:

1. The absorption of light, generating either electron-hole pairs or excitons.
2. The separation of charge carriers of opposite types.
3. The separate extraction of those carriers to an external circuit.
The trouble with homo-junction solar cells

- Only photons with sufficient energy can excite $e^-$ across the band gap $E_g$

- Insufficiently energetic photons with $E_{\text{phot}} < E_g$ will not contribute to the photocurrent generation

- Photons with $E_{\text{phot}} > E_g$ will initially generate energetic excited charge carriers

- Any energy in excess of $E_g$ will be wasted heating up the solar cell through thermalization

Marstein et al, IFE
• Upper limit of homo junction is 33%

<p>| | |</p>
<table>
<thead>
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<tbody>
<tr>
<td>Thermalization ($E &gt; E_g$)</td>
<td>47%</td>
</tr>
<tr>
<td>Transmission ($E &lt; E_g$)</td>
<td>18.5%</td>
</tr>
<tr>
<td>Recombination</td>
<td>1.5%</td>
</tr>
<tr>
<td>Remaining efficiency</td>
<td>33%</td>
</tr>
<tr>
<td>Total</td>
<td>100%</td>
</tr>
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M.C. Beard et al., Nano Letters 7 (2007) p 2506
Shockley-Queisser Limit

1) Smaller bandgaps give higher short circuit current

2) Larger bandgaps give higher open-circuit voltage

3) For the given solar spectrum, an optimum bandgap exists.

- Historical Developments –

- 1839: Photovoltaic effect was first recognized by French physicist Alexandre-Edmond Becquerel.

- 1883: First solar cell was built by Charles Fritts, who coated the semiconductor selenium with an extremely thin layer of gold to form the junctions (1% efficient).

- 1946: Russell Ohl patented the modern solar cell.

- 1954: Modern age of solar power technology arrives – Bell Laboratories, experimenting with semiconductors, accidentally found that silicon doped with certain impurities was very sensitive to light.
DIFFERENT GENERATION OF SOLAR CELLS

(1) First generation – Silicon solar cells

Silicon

- Single crystalline silicon (28%)
- Multicrystalline silicon (21%)
(2) Second generation – Thin film solar cells

- Amorphous silicon (16 %)
- Copper indium gallium diselenide (CIGS) (20 %)
- Cadmium Telluride (CdTe) (17 %)

Diagram showing the layers of a thin film solar cell:
- Ni/Al contacts
- Anti-reflective coating
- Low-resistance ZnO
- High-resistance ZnO
- CdS window layer
- CIGS absorber layer
- Mo back contact
- Soda lime glass

Diagram showing the layers of another thin film solar cell:
- Soda lime glass
- Metal contact
- SnO or ITO
- CdS window layer
- CdTe absorber layer
- Metal back contact
The Falling Price of Utility-Scale Solar Photovoltaic (PV) Projects

- **2010**: Total cost: 21.4 c/kWh
- **2011**: Total cost: 19.8 c/kWh
- **2012**: Total cost: 14 c/kWh
- **2013**: Total cost: 11.2 c/kWh

**2020 Goal**: 6 c/kWh

- **Module**
- **Inverter**
- **Other Hardware (Wires, Fuses, Mounting Racks)**
- **Soft Costs (Permitting, Inspection, Installation)**
(3) Third generation solar cells

- Multijunction solar cells
- Dye sensitized solar cells
- Quantum dot sensitized solar cells
- Organic or polymer solar cells

A multijunction solar cell composed of multiple layers of various semiconductor materials can convert more than 40 percent of incoming sunlight into usable electricity – Photonics Spectra
Conventional Solar Cell
(p-n junction Si)

Excitonic Solar Cell
(DSSC, OPV)

hv

free charges

interface

exciton

a) Schematic diagram of dye-sensitized solar cells
(b) Quantum dot sensitized solar cells

**Advantages** – adjustable band gap, high extinction coefficients, flexible substrate, low cost of materials, better stability, and long life time.

**Schematic diagram of quantum dot sensitized solar cells**

- HOMO: highest occupied molecular orbital
- LUMO: lowest unoccupied molecular orbital
Quantum Confinement effect

Splitting of energy levels in quantum dots due to the quantum confinement effect, semiconductor band gap increases with decrease in size of the nanocrystal.

Source: Sigma-Aldrich
(c) Organic solar cells

![Diagram of an organic solar cell]

**Advantages**
- Low cost
- Light weight
- Easy to fabrication
- Flexible, semi-transparent, etc.

**Layers**
- Cathode
- Photoactive Layer
- Hole Transport Layer (HTL)
- Transparent Anode
- Transparent Substrate
d) Perovskite Solar Cells

• Dyes do not absorb all the incident light, reducing DSSC efficiency.

• In 2009, Miyasaka (Toin U. of Yokohama, Japan) turns to perovskite as possible replacement of the dye and achieved 3.8% efficiency.

• Problem: Liquid electrolyte dissolved away the perovskite within minutes.

0.15 M LiI and 0.075 M I₂ in methoxyacetonitrile
CH₃NH₃PbX – Perovskite ABX₃

Phase Transition (CH₃NH₃PbI₃):
Orthorhombic  →  Tetragonal  →  Cubic
162 K  327 K (54 °C)

The organic ligand is disordered in Tetragonal and Cubic phase.

Figure 1 | Crystal structure. Possible structure of the hybrid perovskite CH₃NH₃PbI₃,Clᵢ. At present, crystallographic data on the precise position of the organic ligands are not available.

Nature. 2013, 12, 1087
J. Mater. Chem. A, 2013, 1, 15628
DSSC with Perovskite

2013, Grätzel sticks with the TiO$_2$ structure and tinkered with the deposition step.

Efficiency: 15%

Nature. 2013, 499, 316
Best Research-Cell Efficiencies

- Multijunction Cells (2-terminal, monolithic)
  - LM = lattice matched
  - IMM = inverted, metamorphic
  - Three-junction (concentrator)
  - Three-junction (non-concentrator)
  - Two-junction (concentrator)
  - Two-junction (non-concentrator)
  - Four-junction (concentrator)
  - Four-junction or more (concentrator)
  - Three-junction (non-concentrator)
  - Three-junction (non-concentrator)

- Single-Junction GaAs
  - Single crystal
  - Concentrator
  - Thin-film crystal

- Crystalline Si Cells
  - Single crystal (concentrator)
  - Single crystal (non-concentrator)
  - Multicrystalline
  - Thick Si film
  - Silicon heterostructures (HIT)
  - Thin-film crystal

- Thin-Film Technologies
  - CIGS (concentrator)
  - CIGS
  - CTe
  - Amorphous Si:H (stabilized)
  - Nano-, micro-, poly-Si
  - Multijunction polycrystalline

- Emerging PV
  - Dye-sensitized cells
  - Perovskite cells
  - Organic cells (various types)
  - Organic tandem cells
  - Inorganic cells (CZTSSe)
  - Quantum dot cells
Best Research-Cell Efficiencies

- Single crystal silicon
- Dye sensitized solar cell
- Cadmium telluride
- Organic photovoltaic
- Amorphous silicon
- Perovskite
- Copper indium gallium selenide
<table>
<thead>
<tr>
<th>Solar cell</th>
<th>Highest reported efficiency (%)</th>
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<tbody>
<tr>
<td>Silicon (single crystal, single cell)</td>
<td>27.6 ±1.0</td>
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<tr>
<td>CIGS (thin film, single cell)</td>
<td>20.3 ±0.6</td>
</tr>
<tr>
<td>CdTe (thin film, single cell)</td>
<td>16.7 ±0.5</td>
</tr>
<tr>
<td>Dye-sensitized (single cell)</td>
<td>11.2 ±0.3</td>
</tr>
<tr>
<td>Organic polymer (single cell)</td>
<td>9.2 ±0.3</td>
</tr>
<tr>
<td>Perovskite</td>
<td>15.0±0.3</td>
</tr>
<tr>
<td>InGaP/GaAs/InGaAs (tandem cell)</td>
<td>42.3 ±2.5</td>
</tr>
</tbody>
</table>
Fourth Generation Solar Cells

Timeline
1G to 4G

Nanoscale,
2013, 5,
8411–8427
Fourth Generation Solar cells

Hybrid - inorganic crystals within a polymer matrix

Nanoscale, 2013, 5, 8411–8427
Organic Solar Cells – Future Applications

PV Charger
Solar Windows
Transportation
Solar Farms
Clothing

Military

Courtesy - SNE Research
DOPED TiO$_2$/PTB7:PC$_{71}$BM BASED INVERTED POLYMER SOLAR CELLS

J. Mater. Chem. 2014, 2, 11426
High performance inverted organic solar cells with solution processed Ga-doped ZnO as an interfacial electron transport layer†

M. Thambidurai,†*a Jun Young Kim,†a Jiyun Song,†a Youngjun Ko,†a Hyung-jun Song,†a Chan-mo Kang,†a N. Muthukumarasamy,†b Dhayalan Velauthapillai†c and Changhee Lee*†a

We demonstrate solution-processed Ga-doped ZnO incorporated as an interfacial electron transport layer into inverted organic solar cells with active layers comprising either PCDTBT or PTB7 mixed with PC71BM. The 5.03 at% Ga-doped ZnO showed the best efficiencies of 5.56% and 7.34% for PCDTBT and PTB7 polymers respectively.
DOPED TiO$_2$/PTB7:PC$_{71}$BM BASED INVERTED POLYMER SOLAR CELLS

Enhanced power conversion efficiency of inverted organic solar cells by using solution processed Sn-doped TiO$_2$ as an electron transport layer

M. Thambidurai,$^{a,*}$ Jun Young Kim,$^{a,*}$ Hyung-jun Song,$^a$ Youngjun Ko,$^a$ N. Muthukumarasamy,$^b$ Dhayalan Velauthapillai,$^c$ Victor W. Bergmann,$^d$ Stefan A. L. Weber$^d$ and Changhee Lee$^a$

We have investigated the photovoltaic properties of inverted solar cells comprising a bulk heterojunction film of thieno[3,4-b]-thiophene/benzodithiophene (PTB7) and [6,6]-phenyl-C$_{71}$-butyric acid methyl ester (PC$_{71}$BM), sandwiched between indium tin oxide (ITO)/Sn-doped TiO$_2$ front and MoO$_3$/aluminum back electrodes. The inverted organic solar cell (IOSC) fabricated with a Sn-doped TiO$_2$ film showed a significantly greater power conversion efficiency of 7.59%, compared to that of the TiO$_2$ film (6.70%). Further studies confirm that the improved morphology and electrical properties of the Sn-doped TiO$_2$ film result in reduced shunt loss and interfacial charge recombination and hence enhanced photovoltaic performance.
High-efficiency inverted organic solar cells with polyethylene oxide-modified Zn-doped TiO$_2$ as an interfacial electron transport layer†

M. Thambidurai,‡,*/a Jun Young Kim,‡,a Youngjun Ko, a Hyung-jun Song,a Hyeonwoo Shin, a Jiyun Song, a Yeonkyung Lee, a N. Muthukumarasamy, b Dhayalan Velauthapillai c and Changhee Lee*/a

High efficiency inverted organic solar cells are fabricated using the PTB7:PC$_{71}$BM polymer by incorporating Zn-doped TiO$_2$ (ZTO) and 0.05 wt% PEO:ZTO as interfacial electron transport layers. The 0.05 wt% PEO-modified ZTO device shows a significantly increased power conversion efficiency (PCE) of 8.10%, compared to that of the ZTO (7.67%) device.
Ongoing solar cell research

Eksperimental:

- Dye Sensitized Solar Cells (DSSC)
- Quantum Dots Sensitized Solar Cells (QDSSC)
- CZTS based Solar Cells
- Organic Solar Cells (OSC)
- Perovskite Solar Cells - initial stages

Computational:

- Simulation study on nano structures for solar cell applications
- Simulation study on Intermediate Bandgap Solar Cells