Molecules to Megawatts: Solar PV Research at UQ

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Co-Director, Centre for Organic Photonics and Electronics
1. UQ owns and operates \(~ 5.6\) MW of solar energy plant: more than any other university in the world
2. UQ has a comprehensive portfolio (>$50M) of clean energy research spanning: fundamental PV science; fundamental battery materials development; power systems engineering and integration; pilot deployment of PV and CST; CST turbine development; biofuels for transport and fine chemicals; energy economics; socio-economics and policy development; resource monitoring and prediction; energy poverty and off-grid systems design; hybrid plant design.

*Molecules to Megawatts (and most things in between)*
UQ Solar: An Attempt to Co-ordinate and Communicate Strategic Intent

UQ SOLAR

GCI Plant

Industrial Portfolio

AGL SFP EIF (AGL / FirstSolar: ARENA)

St Lucia MW Array (P&F)

Thermal Engineering (SMME)

Power Systems & Storage (ITEE)

Energy Economics & Policy (EE)

Fundamentals & Next Gen (SMP/SCMB)

Schools Basics

PV Strategic Research Initiative (SMP/SCMB: ARENA)

CST Strategic Research Initiative (SMP/SMME: ARENA)

ARC & ARENA Projects (SMP/SCMB/SMME/ITE)

Pipeline

Industrial Portfolio

Gatton Clean Energy Community

Bio-algae Pilot with PV

CST CO₂ Sc for Off-grid (SMME: CIF)
Sustainable Advanced Materials @ COPE

**Foci:**
1. Solar cells & photodiodes
2. Bioelectronics
3. Organic sensors
4. Light emitting structures

**Philosophy:**
1. Integrated, multi-disciplinary
2. Molecule to prototype
3. Real world problems
4. Commercialisation & incubation
Our Interests (Next Gen Thin Film Solar Cells)

• **Electro-optics of photoactive diodes and materials**
  Lin et al. *Nature Photonics*, 9 106 (2015);
  Armin et al. *ACS Photonics*, 1 173 (2014);
  Armin et al. *Nature Materials*, 12(7) 593 (2013);
  Lee et al. *Advanced Materials*, 23 766 (2011)

• **Transport physics of disordered semiconductors**
  Stolterfoht et al. *Nature Communications*, In Press (2016);
  Lin et al. *Account of Chemical Research*, 49(3) 545 (2016);
  Stolterfoht et al. *Scientific Reports*, 5 1 (2015);
  Philippa et al. *Scientific Reports*, 4 5695 (2014);

• **Scaling physics: commercially viable solar cells**
  Armin et al. *Advanced Energy Materials*, 5 1401221 (2015);
Different Types of Thin Film Solar Cells?

Lin, Armin et. al. *Account of Chemical Research*, 49(3) 545 (2016)
Thin Film Organic Solar Cell: Really Simple Architectures

(A) Bilayer Device
- Metal contact
- Hole blocking layer
- Acceptor
- Donor
- Electron blocking layer
- Transparent Conductor
- Transparent substrate

(B) Bulk heterojunction Device
- Metal contact
- Hole blocking layer
- Donor-Acceptor blend
- Electron blocking layer
- Transparent conductor
- Transparent substrate
Organic Semiconductors ($n$-and-$p$-type): Excitonic at RT

- PC$_{71}$BM
- rr-P3HT
- $p$-DTS(FBTTh$_2$)$_2$
- PC$_{60}$BM
- PCDTBT
Organic Photodiode or Solar Cell: Basic Mode of Action

Important:
- Static dielectric constant $< 5$
- Excitonic ($\sim 0.2 - 0.5 \text{eV } E_B$)
- Molecular junction
- Transport physics “hopping”
- $\mu < 10 \text{ cm}^2/\text{Vs}$
- Recombination bimolecular

Also Important:
- Power conversion efficiencies $> 12\%$
- Must be encapsulated ($\text{O}_2$ and $\text{H}_2\text{O}$)
- As yet, have not been scaled (modules)
- Physics is really interesting
- Closest to artificial photosynthesis?

Fan et al. *Advanced Energy Materials*, 3(1) 54 (2013);
Lee et al. *Advanced Materials*, 23 766 (2011)
Electro-optics

- Optical field distribution (thin-film, low finesse cavity)

![Graph showing optical field distribution](image)

- Chemical structures of PCDTBT and PC$_{70}$BM

1:4
Junction Thickness – Optical Field Effects

(b)

EQE [%]

BHJ layer thickness
- 280 nm
- 115 nm
- 72 nm
- 42 nm

Wavelength [nm]

Armin et al. *ACS Photonics*, 1 173 (2014);
Slower carrier controls:
- Recombination and extraction efficiency; AND
- Charge generation yield due to an entropic driving force.
“Big” Organic Solar Cells

Relevant Scaling Physics:
- Defect density scales exponentially with active area;
- Transparent anode sheet resistance limits collection path;
- $R_{sh}$ impacts recombination coefficient and deviation current.
Model Planar \((\text{CH}_3\text{NH}_3\text{PbI}_3)\) Solar Cell

“it does not get any simpler than this”

\(\text{p- and } n\text{-type interlayers } \sim 10 \text{ nm}: \text{ not transport layers but work function modifiers}

“Metal-Insulator-Metal homojunction”
Internal quantum efficiency (IQE)

Predominantly Non-excitonic Branching Fraction at RT? (low frequency $\varepsilon'$ and optical frequency n,k)

$\text{CH}_3\text{NH}_2\text{PbI}_3$

Direct measurement of the exciton binding energy and effective masses for charge carriers in organic-inorganic tri-halide perovskites

Atsuhiro Miyata, Anatolie Mitioglu, Paulina Plochocka, Oliver Portugall, Jacob Tse-Wei Wang, Samuel D. Stranks, Henry J. Snaith and Robin J. Nicholas

Solar cells based on the organic-inorganic tri-halide perovskite family of materials have shown significant progress recently, offering the prospect of low-cost solar energy from devices that are very simple to process. Fundamental to understanding the operation of these devices is the exciton binding energy, which has proved both difficult to measure directly and controversial. We demonstrate that by using very high magnetic fields it is possible to make an accurate and direct spectroscopic measurement of the exciton binding energy, which we find to be only 16 meV at low temperatures, over three times smaller than has been previously assumed. In the room-temperature phase we show that the binding energy falls to even smaller values of only a few millielectronvolts, which explains their excellent device performance as being due to spontaneous free-carrier generation following light absorption. Additionally, we determine the excitonic reduced effective mass to be 0.104me, (where me is the electron mass), significantly smaller than previously estimated experimentally but in good agreement with recent calculations. Our work provides crucial information about the photophysics of these materials, which will in turn allow improved optoelectronic device operation and better understanding of their electronic properties.

“Irrespective of the exact value, such a low \( E_B \) (C.f. Si: 15.0 meV; GaAs: 4.2 meV; CdTe: 10.5 meV) dictates that perovskite solar cells should be predominantly non-excitonic at room temperature”

\[ 1.7 \text{ meV} < E_B < 2.1 \text{ meV} \]
Thin Film Electro-Optics (Again)

[Graph showing light intensity (|E|^2) vs. distance from Glass/ITO interface (nm) for different wavelengths (400 nm, 500 nm, 600 nm, 700 nm).]

[Graph showing EQE (%) vs. wavelength (nm) for Beer-Lambert and cavity regions for different thicknesses (180 nm, 260 nm, 340 nm, 370 nm, 430 nm, 520 nm).]
Experiment versus Model

![Graph showing the comparison between experiment and model results for Jsc (mA/cm^2) versus thickness (nm). The graph includes a line for the model and markers for the experiment data points. The x-axis represents thickness in nanometers, ranging from 100 to 600, and the y-axis represents Jsc in mA/cm^2, ranging from 12 to 24. The shaded area highlights a specific range of thickness.]
The Optimised Outcome

Glass/ITO (80 nm)/PEDOT:PSS (15 nm)/PCDTBT (5 nm)/Junction (370 nm)/PC60BM (10 nm)/Ag (100 nm)

Hysteresis Free & $V_{oc}$ dependent upon electrode work function offset
What next? Vincent’s sugar cubes.
Scaling ......
A Culture Changing Project: The UQ MW Array

Key Statistics:
- 9.3 GW hr in 56 months;
- 17.8% Capacity Factor;
- 8.9MKg of CO₂ mitigated;
- > 1500 visitors;
- ~ $1.2M in savings;
- On-track for 8-10 year payback;
- Big research potential;
- Data being used by industry, government and research organisations;
- Still the largest roof-top PV system in AU!
AGL Solar PV Project
$166.7M ARENA Funding
$65M NSW Gov Funding
$40.7M EIF Funding
Gatton Solar Research Facility (PC February 2015: 5.33 GWh to 13th February 2016)

- 3.275MW (630kW SAT; 630kW DAT; 2.015 FA) ~37,000 CdTe First Solar Panels
- Research Building, Visitor Centre, Data Hub and Servers
- 600kW, 760kWh Kokam Lithium Polymer Battery
- Bespoke Central Supervisory System with Integrated Battery Management Systems

PV Array Performance

Array Energy (MWh):
- FT1: 4.27
- FT2: 4.40
- FT3: 4.25
- SAT: 4.82
- DAT: 5.19
- Total = 22.93 MWh (30.3% CF)

19th March 2015
BESS System Specification

- 600 kW, 760 kWh Lithium Polymer BESS
- 576~748 V DC
- Interfaced by 4x300 kVA VACON Inverters with 415 V, 3 ph AC output
- Capable of sourcing/sinking reactive power at 0.9 power factor
Battery Research Agenda

How do we store excess PV energy?

While BESS is charged and discharged, how is its capacity and cycle-life affected?

How do we shave/shift load using stored energy?

How can we best utilise BESS as a critical asset?

How do we deal with fluctuation/intermittency issues using BESS?
A Few Take Home Messages

1. UQ Solar Power research agenda broadly spans PV, CST, molecules to MW, panel to policy

2. UQ philosophy of ‘learning through doing’ led to 5.6 MW under ownership and operations – a university as a power company with a change in philosophy

3. Systems understanding informs all aspects of our agenda – next generation materials and cell design through to power systems and markets

4. This approach drives impact and allows a wide stakeholder base to be engaged

5. QRET Issues Paper released yesterday – viable pathway to a 50% target for QLD
The Team – Across the Discipline Divides

- **COPE**: Ardalan Armin, Vincent Lin, Martin Stolterfoht, Helen Jin, Mike Hambsch, Paul Burn

- **UQ Solar (& GCI)**: Jan Alam, Ruifeng Yan, Craig Froome, Vince Garrone, John Foster, Lynette Molyneaux, Liam Wagner (Griffith), Phil Wild, Tapan Saha, Shane Goodwin, Gemma Clayton, Ove Hoegh-Guldberg

- **P&F and Gatton PCG**
  - Geoff Dennis (QUT), Adrian Mengede, Steve Ingram, Andrew Wilson, Carlos Dimas, Gatton Community

- **Partners**
  - Trina
  - AGL & First Solar
  - Hutchins & McNab
  - MPower
  - Provecta
  - Department of Education (Canberra)
  - ARENA, QLD State Government
Exciton binding energy – low frequency or optical ε’?

Solution to the Wannier (Mott) equation:

\[ E_B = \frac{\mu}{m_0 \varepsilon^2} \frac{1}{2} \frac{m_0 e^4}{(4\pi \varepsilon_0 \hbar)^2} \]

Real part of dielectric constant screens the electric field – via the polarisation of the lattice (excitation of optical phonons) or polarisation of valence electrons: for CH$_3$NH$_3$PbI$_3$ exciton separation >> lattice constant and static ε must be used.

\[ \frac{4 \pi^2 \hbar^4 \varepsilon^2 \varepsilon_0^2}{\mu^3 e^2} = c_0 \]

\[ c_0 \sim 1.35 \times 10^{-6} \text{ eV/T}^2 \text{ to } 2.7 \times 10^{-6} \text{ eV/T}^2 \]

\[ [\text{Roth et al. Phys. Rev. 114, 90-103 (1959)}] \]

\[ [\text{Tanaka et al. Solid State Commun. 127, 619-623 (2003)}] \]

\[ 1.7 \text{ meV} < E_B < 2.1 \text{ meV} \]

\[ [\text{D’Innocenzo et al. Nature Commun. 5, 3586 (2014): \sim 50 \text{ meV}}] \]

\[ [\text{Frost et al. Nano Lett. 14, 2584-2590 (2014): < 1 \text{meV}}] \]
$n$-and-$p$-type electrode interlayers

- PCDTBT
- PCPDTBT
- P3HT
- DPP-DTT
- PC60BM
- PEDOT:PSS
**Electrode interlayers**

Energy (eV)

- P3HT: -5.0
- PCPDTBT: -5.0
- DPP-DTT: -5.2
- PCDTBT: -5.3
- CH$_3$NH$_3$PbI$_3$: -3.9
- PC60BM: -4.2

Photoemission Spectroscopy in Air
3. Electrode work function difference influences $V_{oc}$

<table>
<thead>
<tr>
<th>Material</th>
<th>$J_{sc}$ (mA/cm²)</th>
<th>$V_{oc}$ (V)</th>
<th>FF</th>
<th>PCE (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PCDTBT</td>
<td>15.9±0.7</td>
<td>1.03±0.01</td>
<td>0.66±0.05</td>
<td>10.9±0.8</td>
</tr>
<tr>
<td>DPP-DTT*</td>
<td>13.3</td>
<td>1.00</td>
<td>0.74</td>
<td>9.8</td>
</tr>
<tr>
<td>P3HT</td>
<td>14.2±0.9</td>
<td>0.70±0.10</td>
<td>0.78±0.03</td>
<td>8.5±0.8</td>
</tr>
<tr>
<td>PCPDTBT</td>
<td>13.0±0.8</td>
<td>0.88±0.06</td>
<td>0.69±0.04</td>
<td>7.8±0.8</td>
</tr>
</tbody>
</table>
Hysteresis: interfacial phenomenon?

Scan rate at different times.

- Scan from -1 V to 1.2 V
- Scan from 1.2 V to -1 V

Scan rate: 0.1 V/s, 0.05 V/s, 0.2 V/s

Time: t=0, t=4 months
Cell & Bank Configuration

Cells
1. Kokam Manufactured Superior Lithium Polymer Battery cells
2. Rated cell capacity: 75 Ah
3. Cell voltage: 2.7 V to 4.1 V, average 3.7 V
4. Maximum Continuous Charging Current: 2C (150 A) at 23±3 °C
5. Maximum Continuous Discharging Current: 5C (375 A) at 23±3 °C
6. Peak Discharging Current: 8C (600 A), <10 sec and with >50% SoC
7. Cycle-Life: 4000 Cycles at 80% DoD, 1C (Charge) /1C (Discharge).
8. Charging Temperature: 10 to 35 °C
9. Discharging Temperature: -10 to 55 °C

Banks
1. 2 Banks; 4 Racks per Bank; 10 Series Modules per Rack; 2 Parallel Strings of 18 Series Cells per Module
2. Battery Management System (BMS) at Module, Rack, and Bank Level
3. Rack and Bank level BMS can provide critical information e.g. average cell voltage and temperature
BMS-CCS Integration & Initial Commissioning Learnings

Integration
1. BESS Programmable Logic Controller (PLC) is integrated with the Central Supervisory System (CSS) PLC
2. CSS collects and processes information on campus load and PV generation to issue commands for BESS operation

Commissioning Learnings
1. Energy efficiency measured from full charge-discharge cycle test: Bank A - 88.6%, Bank B - 89.0%
2. With proper air conditioning system, average cell temperature remained within 35 °C at typical Gatton ambient
3. Tripping of inverters were observed due to high heatsink temperature (80 °C): correct cooling and ventilation system is required and under modification
4. BMS under CSS control!