Molecules to Megawatts: Solar PV Research at UQ

gciQ Global Change Institute

COPE

UQ SOLAR
Australia's largest flat-panel photovoltaic installation is here.

Paul Meredith

Director UQ Solar, Global Change Institute
Co-Director, Centre for Organic Photonics and Electronics

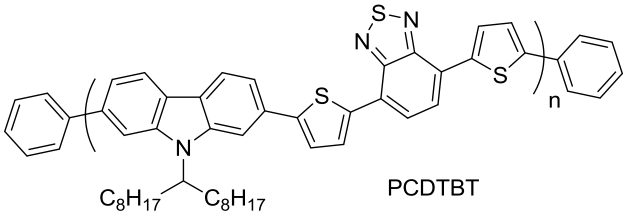
THE UNIVERSITY OF QUEENSLAND
AUSTRALIA

ACAP

Setting the Scene

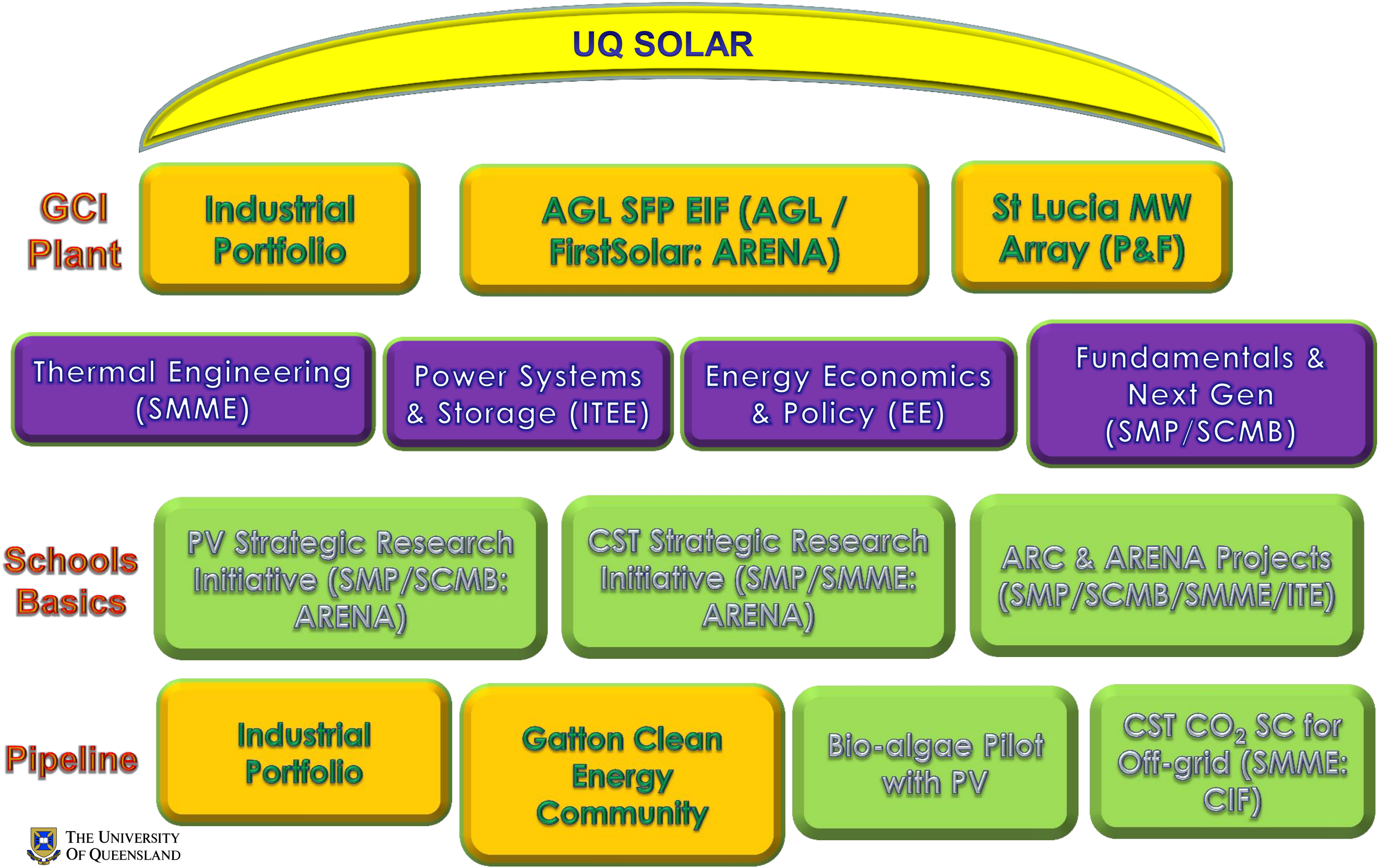
1. UQ owns and operates ~ 5.6 MW of solar energy plant: more than any other university in the world
2. UQ has a comprehensive portfolio (>$50M) of clean energy research spanning: fundamental PV science; fundamental battery materials development; power systems engineering and integration; pilot deployment 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)



PCDTBT

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)

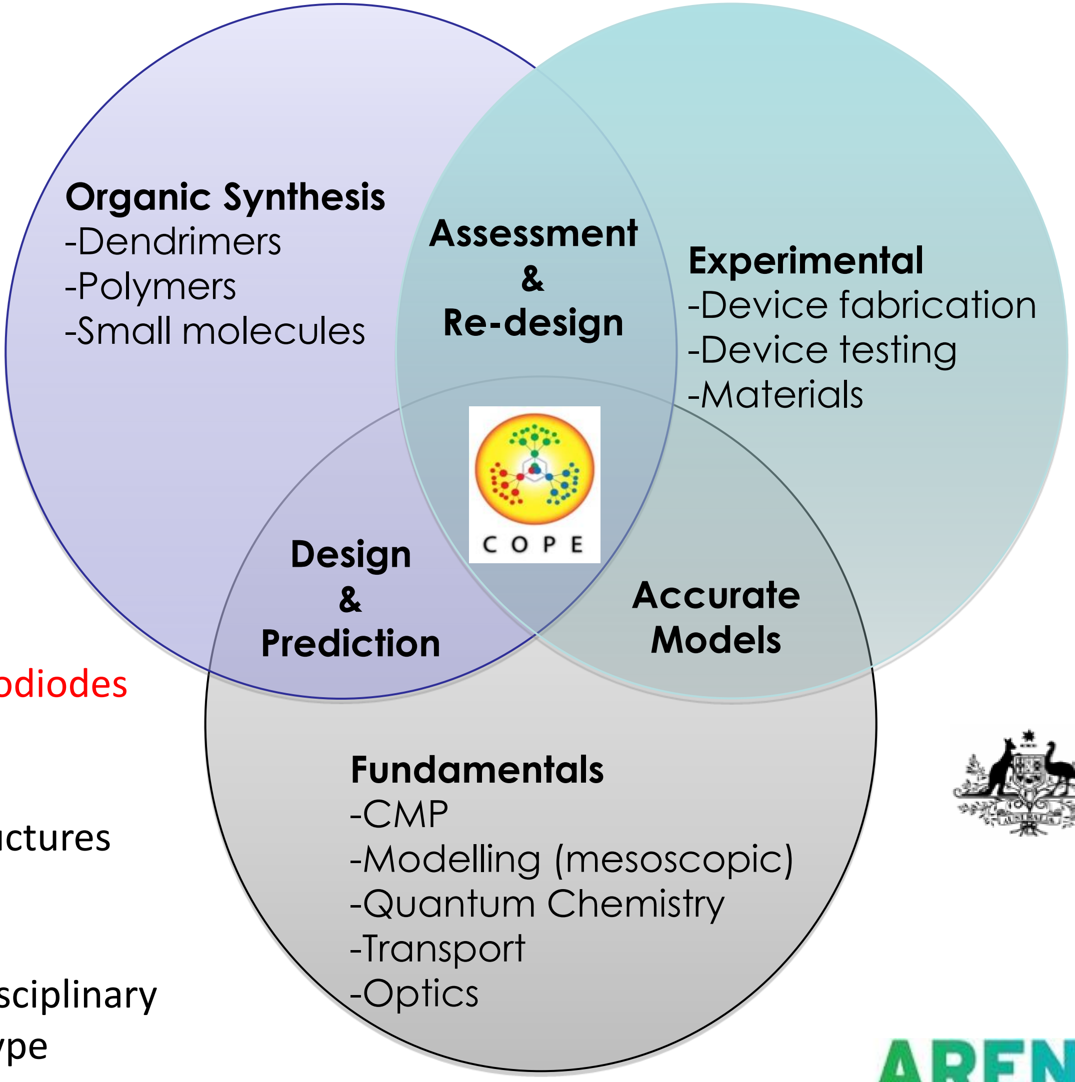
Schools Basics

- 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 CO_2 SC for Off-grid (SMME: CIF)

Sustainable Advanced Materials @ COPE



Organic Synthesis
-Dendrimers
-Polymers
-Small molecules

Assessment
&
Re-design

Experimental
-Device fabrication
-Device testing
-Materials

COPE

Design
&
Prediction

Accurate
Models

Fundamentals
-CMP
-Modelling (mesoscopic)
-Quantum Chemistry
-Transport
-Optics

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
5. Commercialisation & incubation

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First Solar.

CSIRO

The University Of Queensland
Australia

Australian Government
Australian Research Council

Queensland Government

ARENA

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)

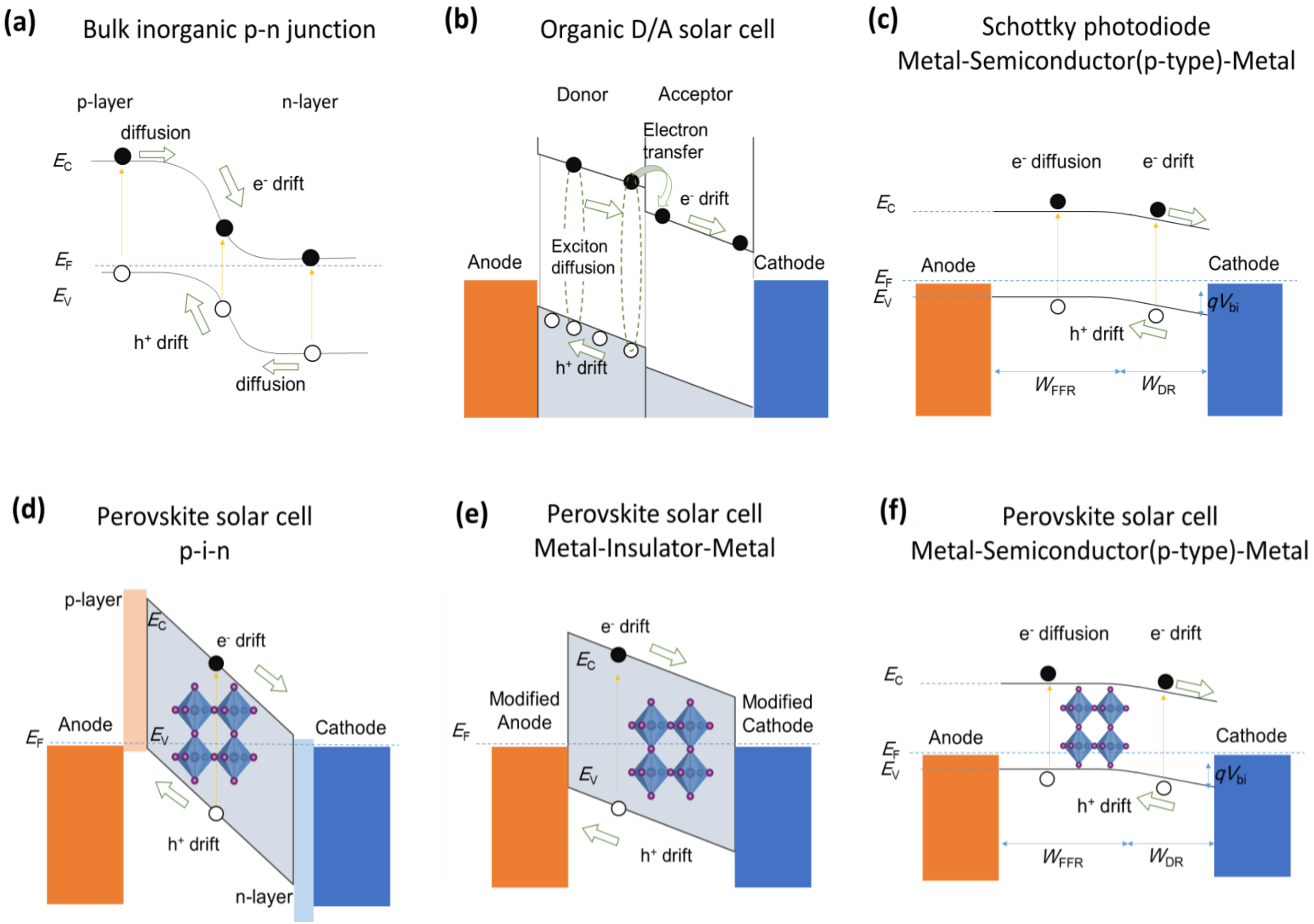
- Transport physics of disordered semiconductors

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);
Armin et al. *Advanced Energy Materials,* **4(4)** 1300954 (2014)

- Scaling physics: commercially viable solar cells

Armin et al. *Advanced Energy Materials,* **5** 1401221 (2015);
Jin et al. *Advanced Materials,* **24(19)** 2572 (2011)

Different Types of Thin Film Solar Cells?

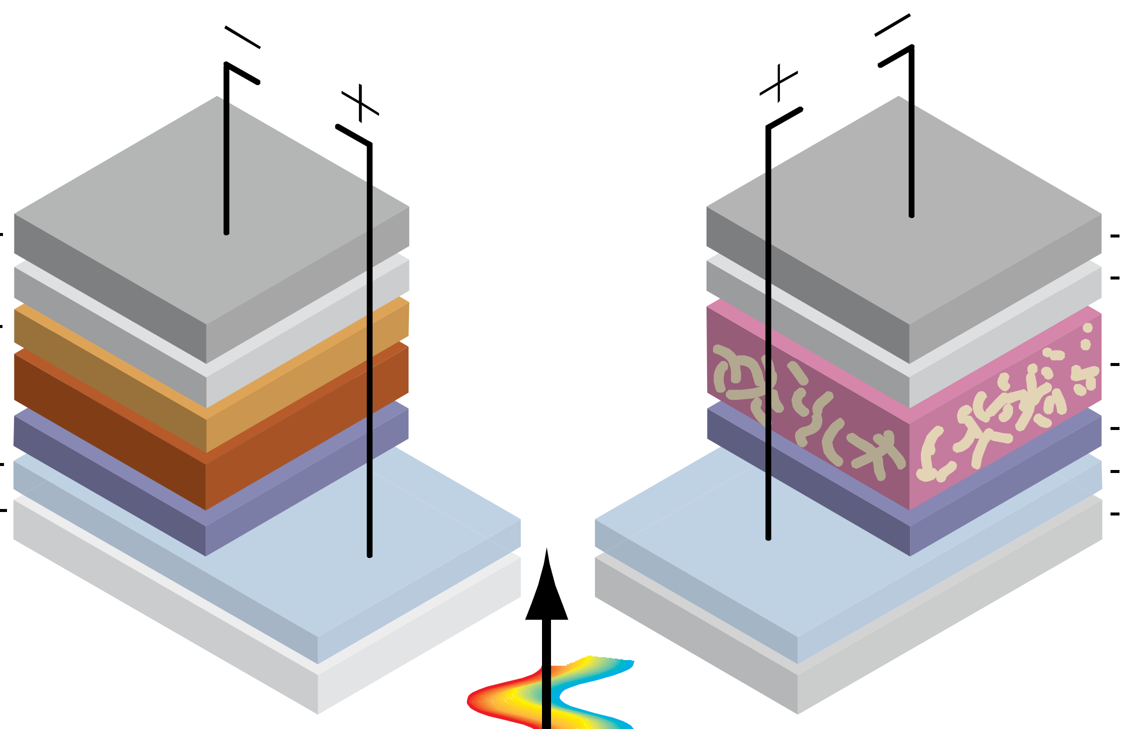


Lin, Armin et. al. *Account of Chemical Research,* **49(3)** 545 (2016)

Thin Film Organic Solar Cell: Really Simple Architectures

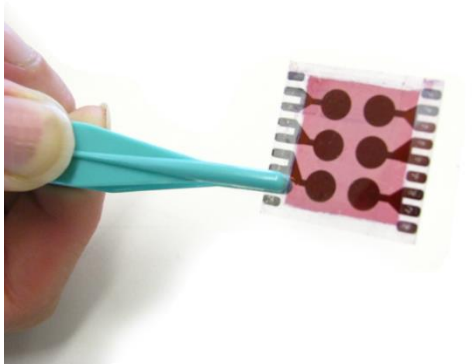
(A) Bilayer Device

(B) Bulk heterojunction Device

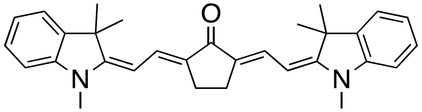


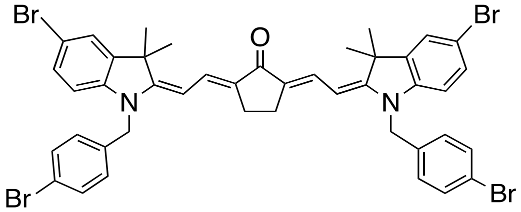
Metal contact ---
Hole blocking layer ---
Acceptor ---
Donor ---
Electron blocking layer ---
Transparent Conductor ---
Transparent substrate ---

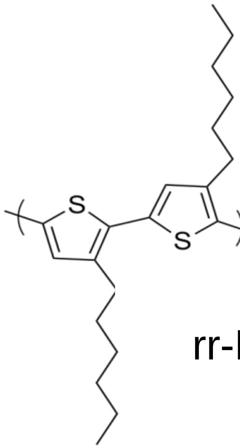
--- Metal contact
--- Hole blocking layer
--- Donor-Acceptor blend
--- Electron blocking layer
--- Transparent conductor
--- Transparent substrate



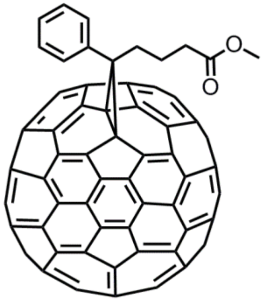
Organic Semiconductors (*n*-and-*p*-type): Excitonic at RT



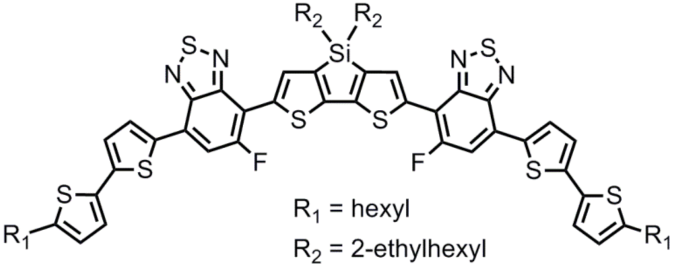




rr-P3HT



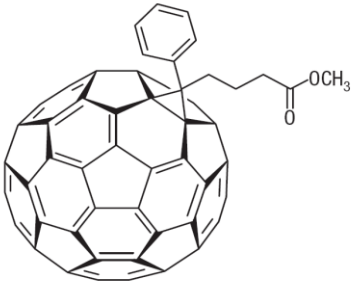
$PC_{71}BM$



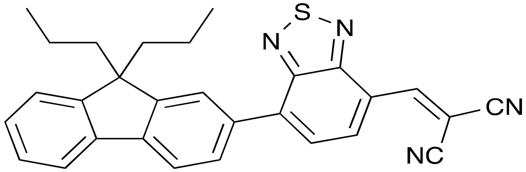
R_1 = hexyl

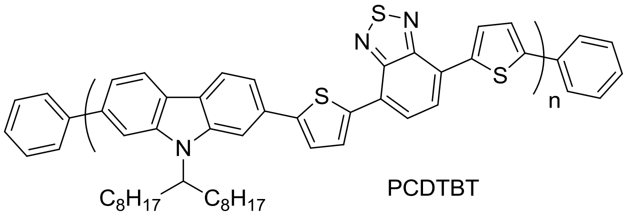
R_2 = 2-ethylhexyl

p-DTS(FBTTh$_2$)$_2$



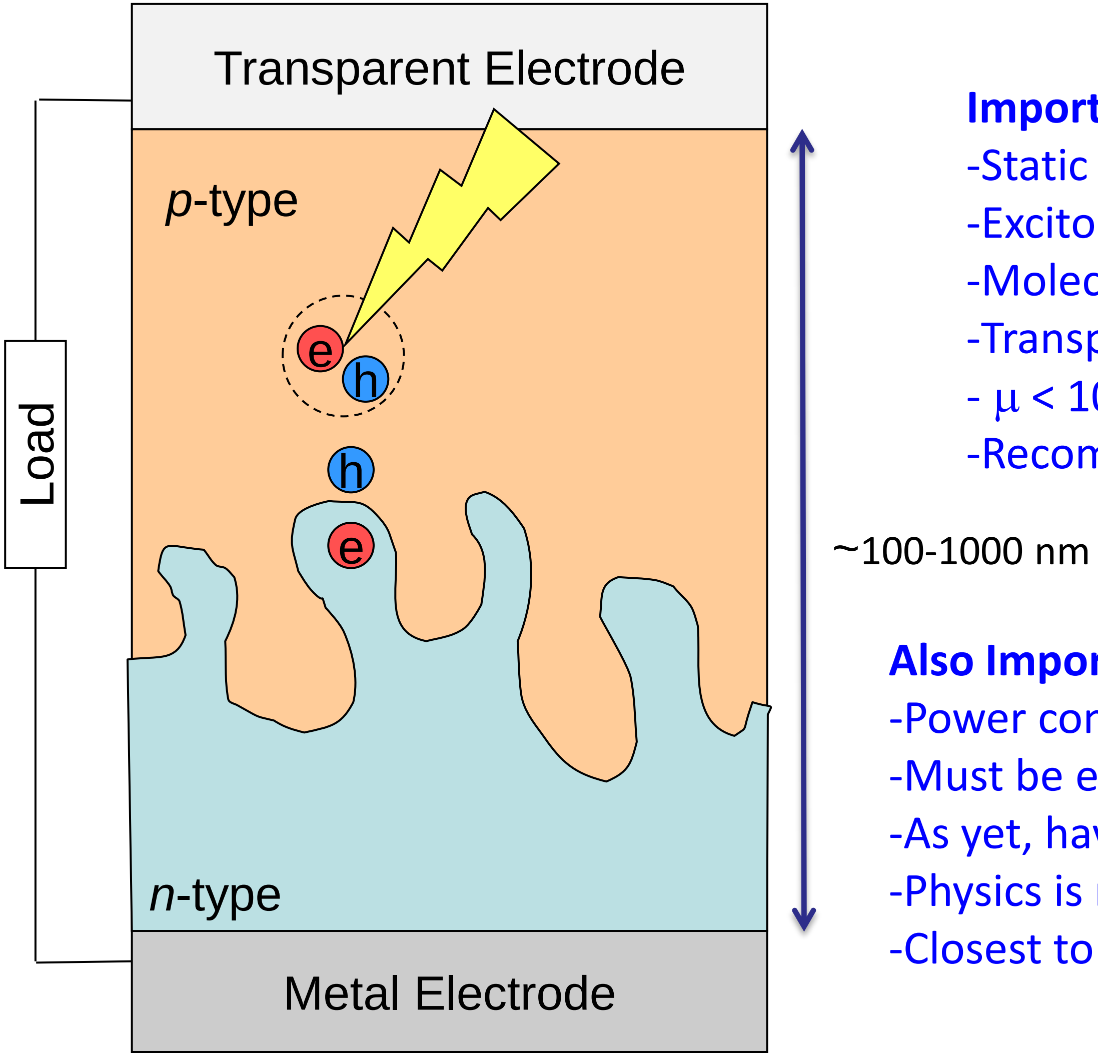
$PC_{60}BM$





PCDTBT

Organic Photodiode or Solar Cell: Basic Mode of Action



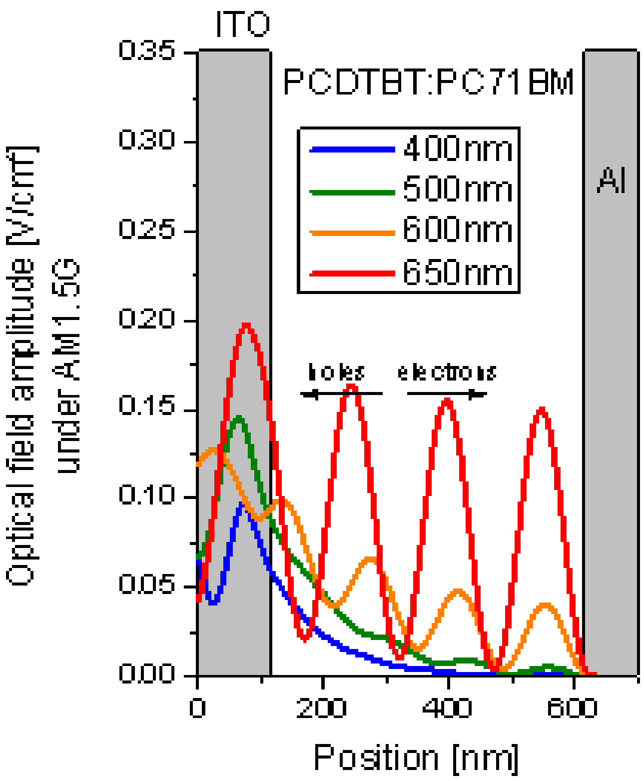
Important:
-Static dielectric constant < 5
-Excitonic (~0.2-0.5eV E_B)
-Molecular junction
-Transport physics “hopping”
- $\mu < 10\ cm^2/Vs$
-Recombination bimolecular

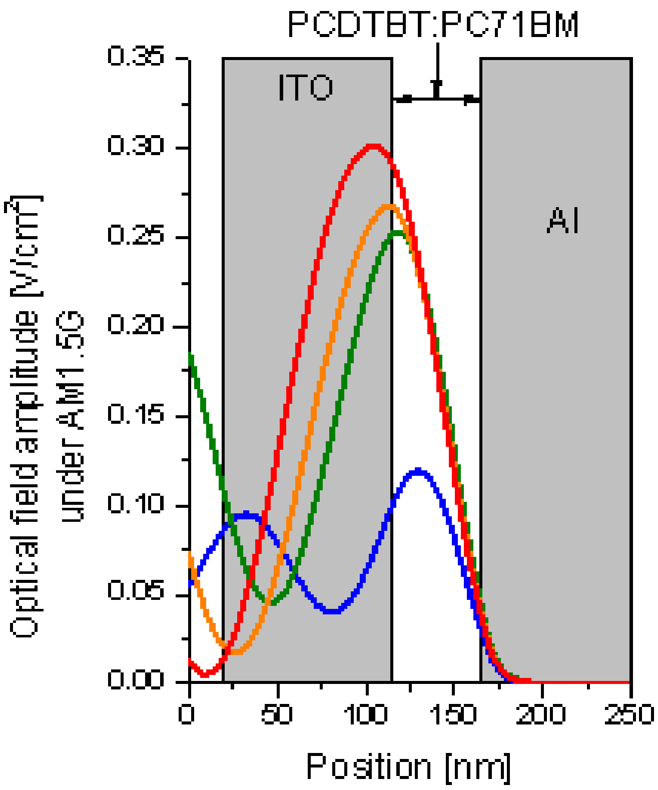
Also Important:
-Power conversion efficiencies > 12%
-Must be encapsulated (O_2 and H_2O)
-As yet, have not been scaled (modules)
-Physics is really interesting
-Closest to artificial photosynthesis?

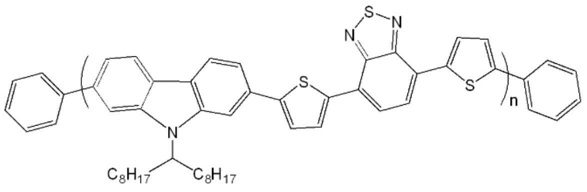
Fan et al. *Advanced Energy Materials*, **3(1)** 54 (2013);
Lee et al. *Advanced Materials*, **23** 766 (2011)

Electro-optics

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

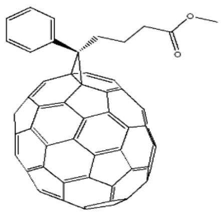






PCDTBT

1:4



$PC_{70}BM$

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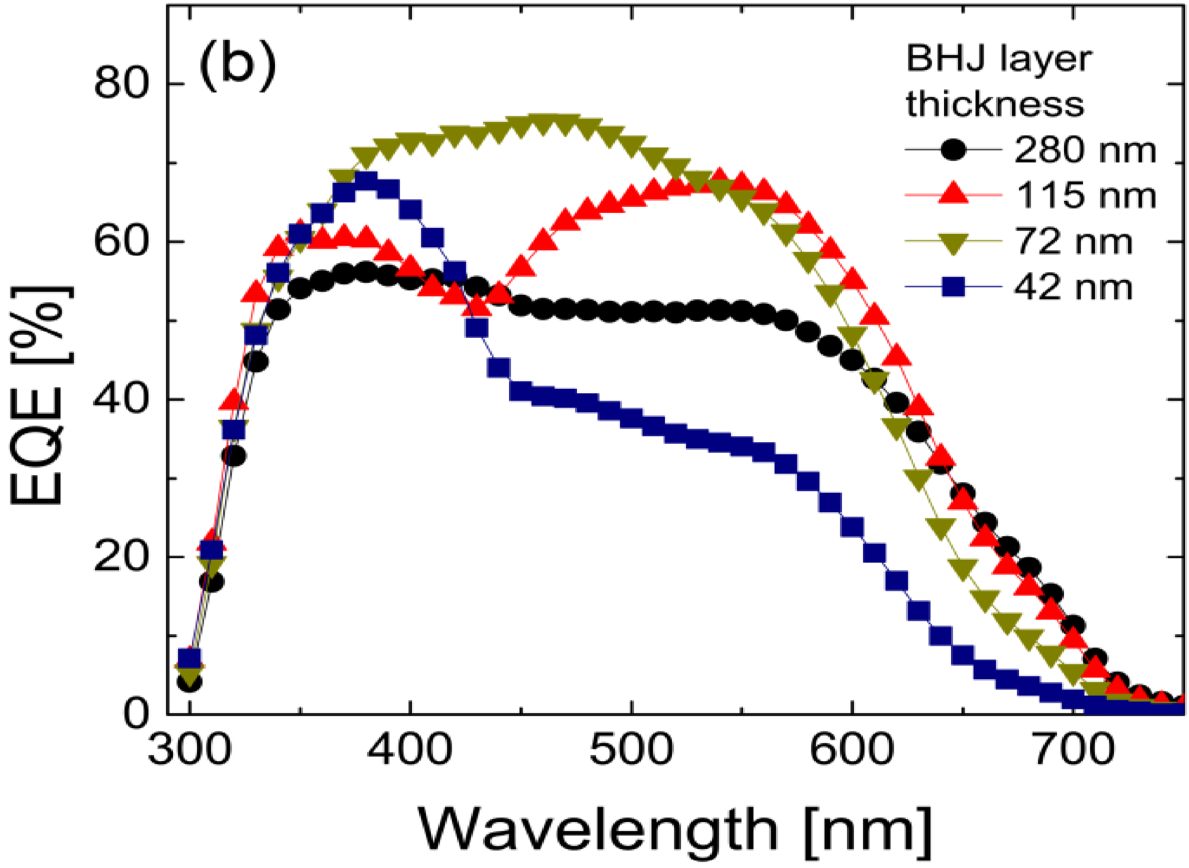
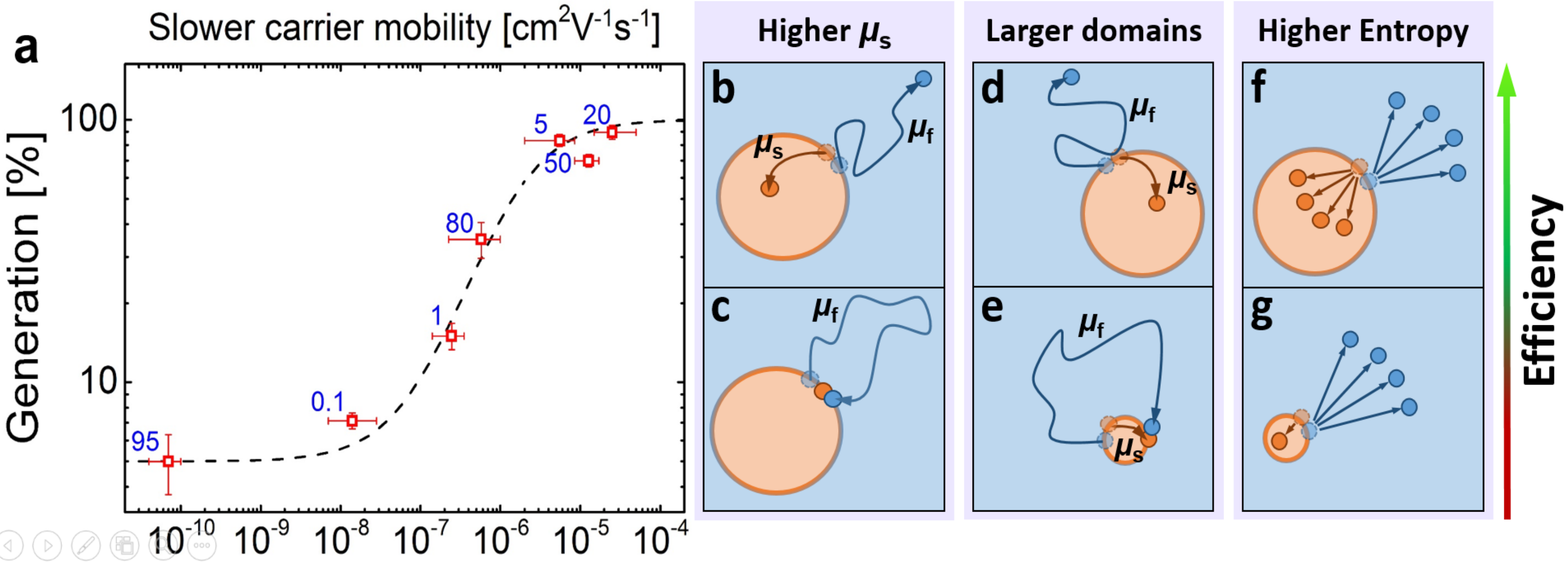
Junction Thickness – Optical Field Effects



Armin et al. *ACS Photonics*, **1** 173 (2014);
Armin et al. *Nature Materials* **12(7)** 593 (2013)

Charge Generation and Transport

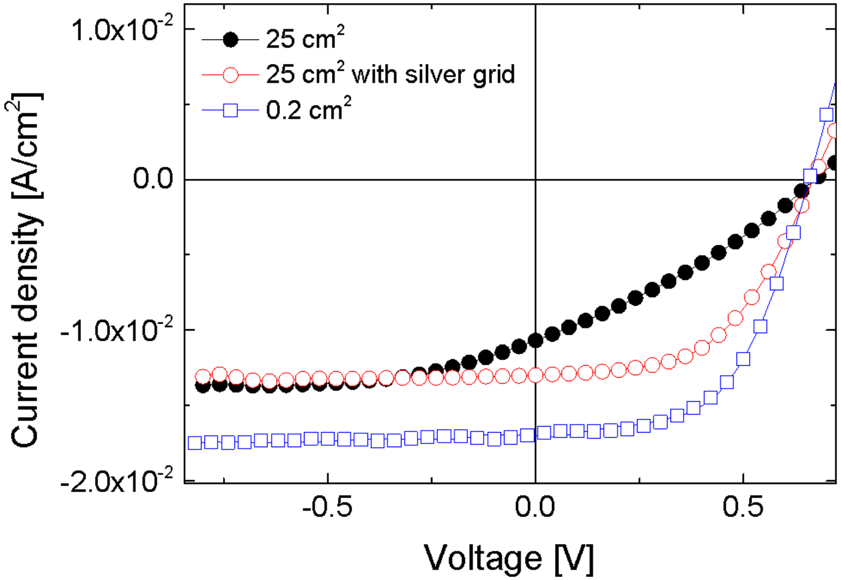


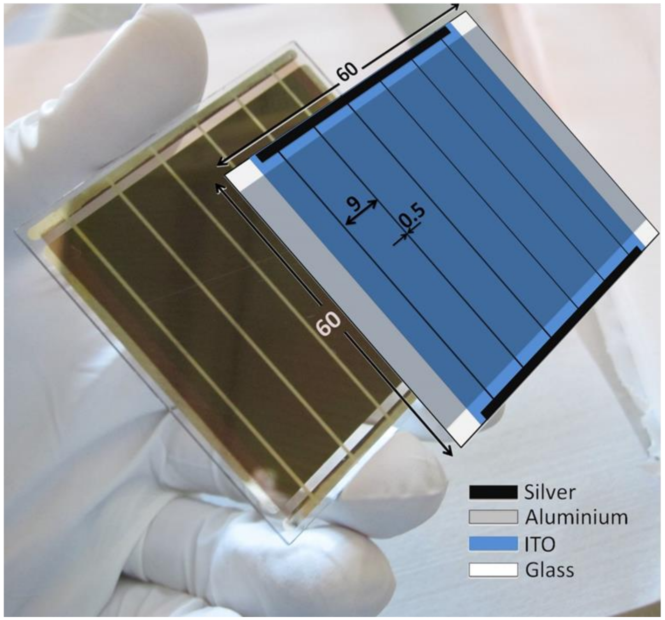
Slower carrier controls:

- Recombination and extraction efficiency; AND
- Charge generation yield due to an entropic driving force.

Stolterfoht et al. *Nature Communications*, In Press (2016)

“Big” Organic Solar Cells





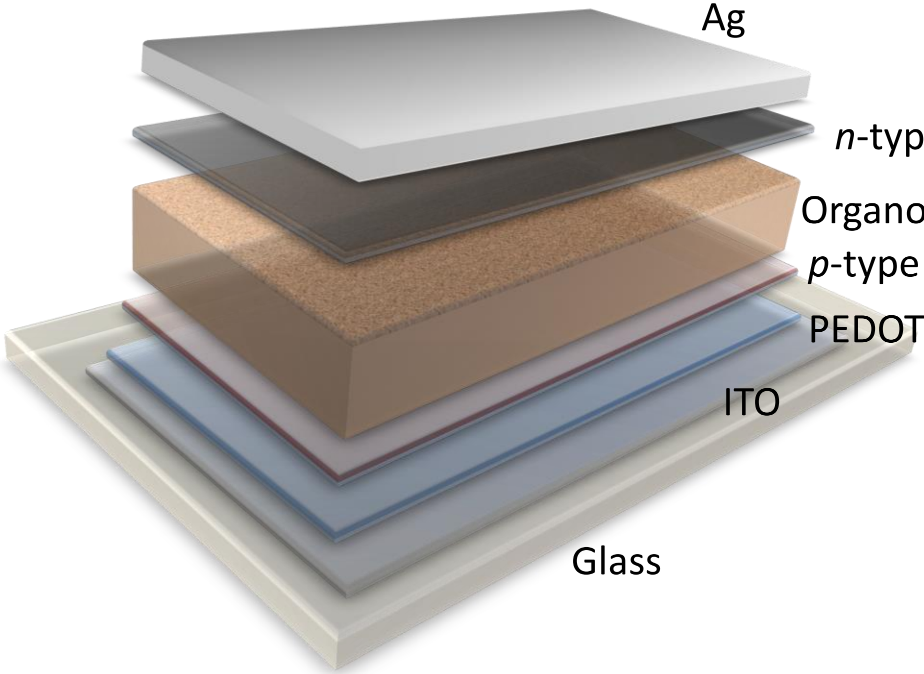
Relevant Scaling Physics:

- Defect density scales exponentially with active area;
- Transparent anode sheet resistance limits collection path;
- R_{sh} impacts recombination coefficient and deviation current.

Armin et al. *Advanced Energy Materials* **5** 1401221 (2015)

Model Planar ($CH_3NH_3PbI_3$) Solar Cell

“it does not get any simpler than this”



Ag

n-type interlayer

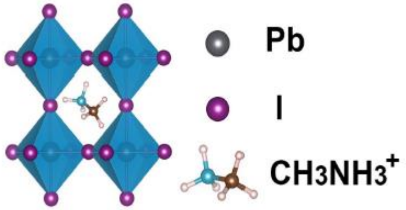
Organohalide Perovskite Homojunction

p-type interlayer

PEDOT:PSS

ITO

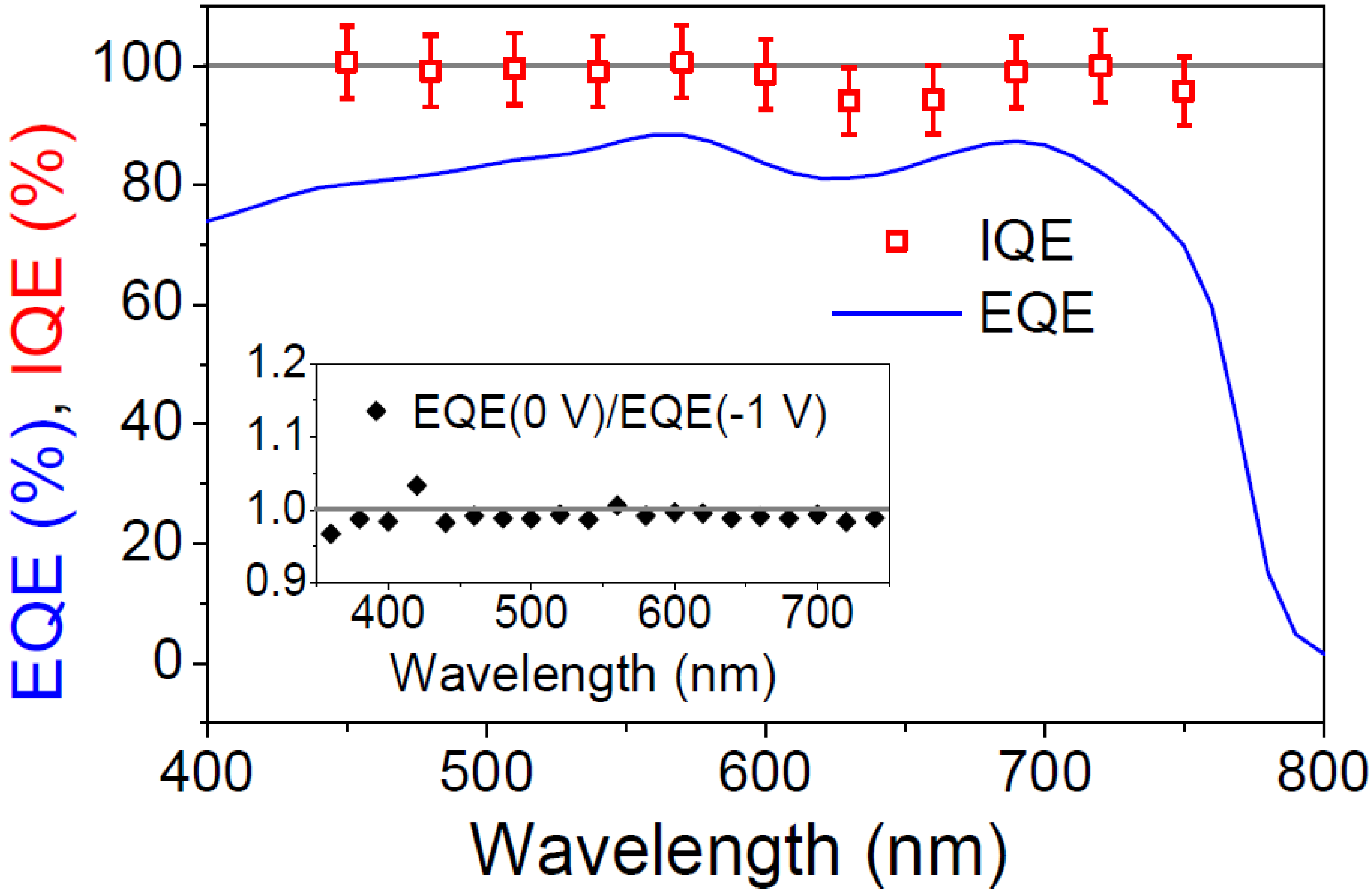
Glass



Perovskite: ABX_3
e.g. $CaTiO_3$

p-and-*n* type interlayers ~ 10 nm: not transport layers but work function modifiers
“Metal-Insulator-Metal homojunction”

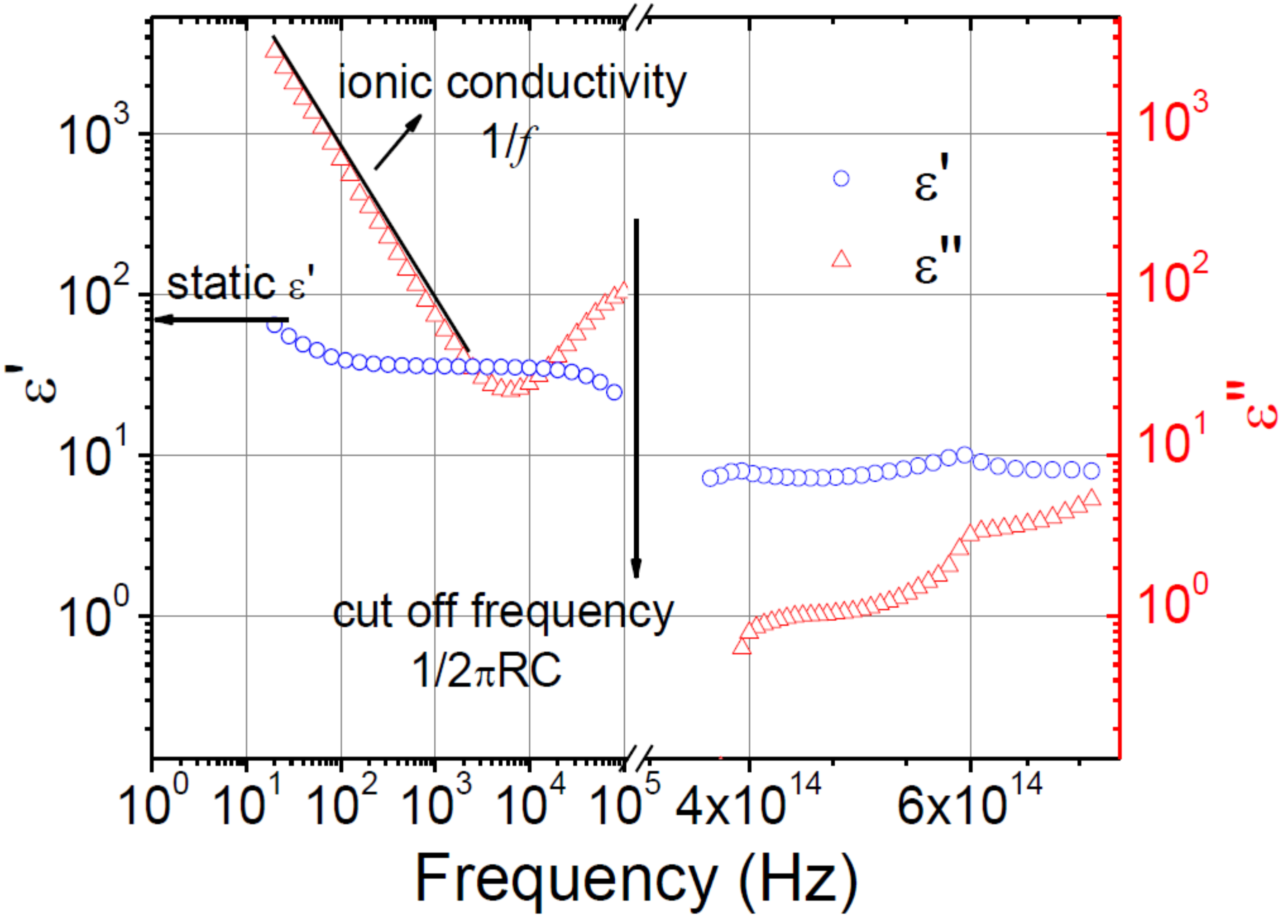
Internal quantum efficiency (IQE)



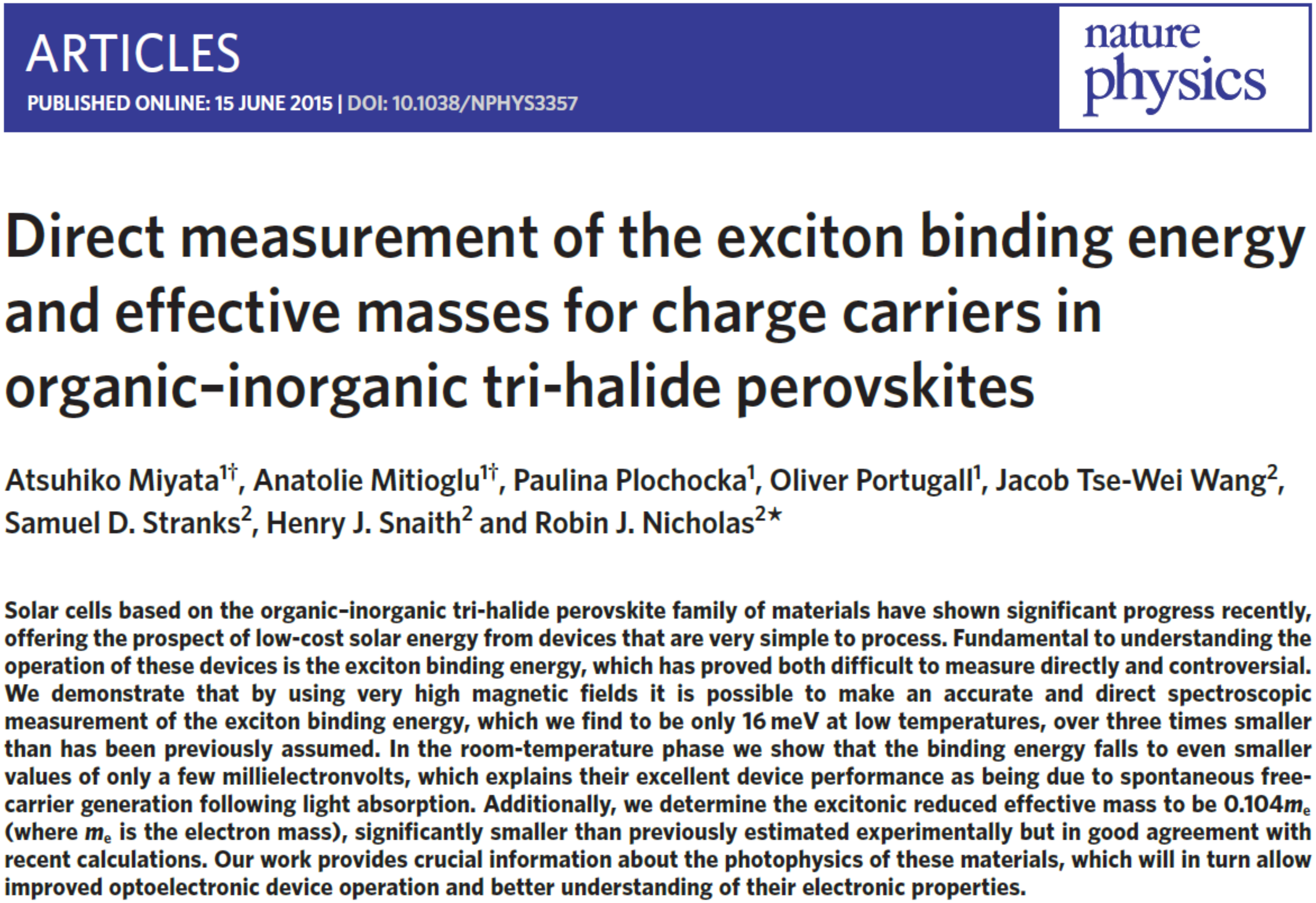
Lin, Armin et. al. *Nature Photonics*, **9** 106 (2015)

Predominantly Non-excitonic Branching Fraction at RT?
(low frequency ε’ and optical frequency n,k)

$CH_3NH_3PbI_3$



n, k data available at: http://www.physics.uq.edu.au/cope/



ARTICLES
PUBLISHED ONLINE: 15 JUNE 2015 | DOI: 10.1038/NPHYS3357
nature physics

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

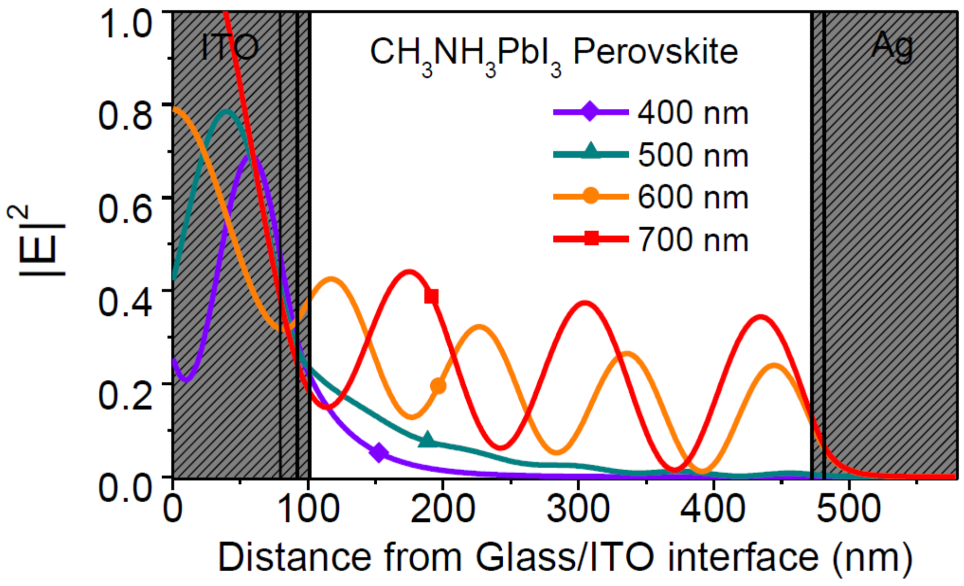
Atsuhiko Miyata[1†], Anatolie Mitioglu[1†], Paulina Plochocka[1], Oliver Portugall[1], Jacob Tse-Wei Wang[2], Samuel D. Stranks[2], Henry J. Snaith[2] and Robin J. Nicholas[2*]

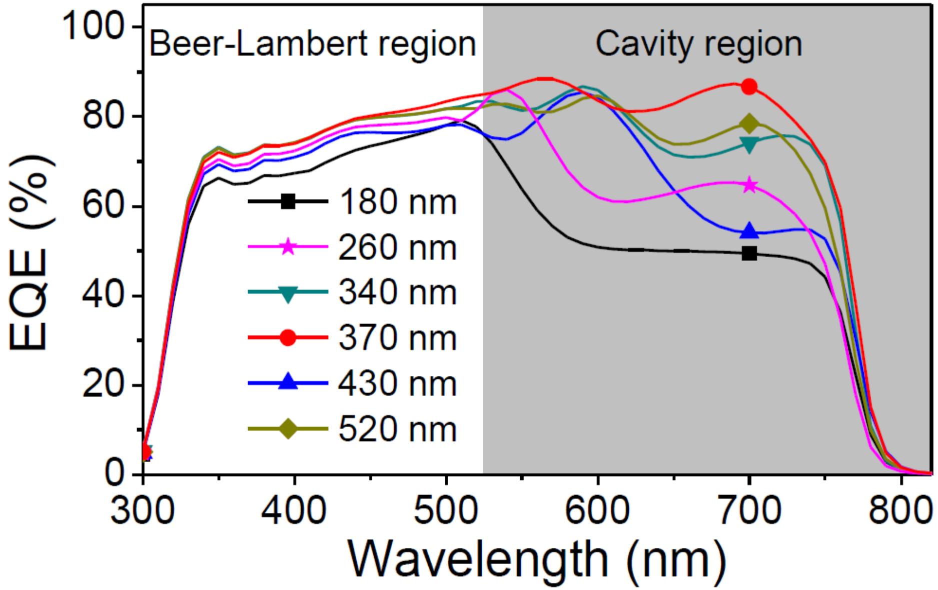
Solar cells based on the organic–inorganic tri-halide perovskite family of materials have shown significant progress recently, offering the prospect of low-cost solar energy from devices that are very simple to process. Fundamental to understanding the operation of these devices is the exciton binding 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 0.104m_e (where m_e 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"

$$1.7\ meV < E_B < 2.1\ meV$$

Thin Film Electro-Optics (Again)





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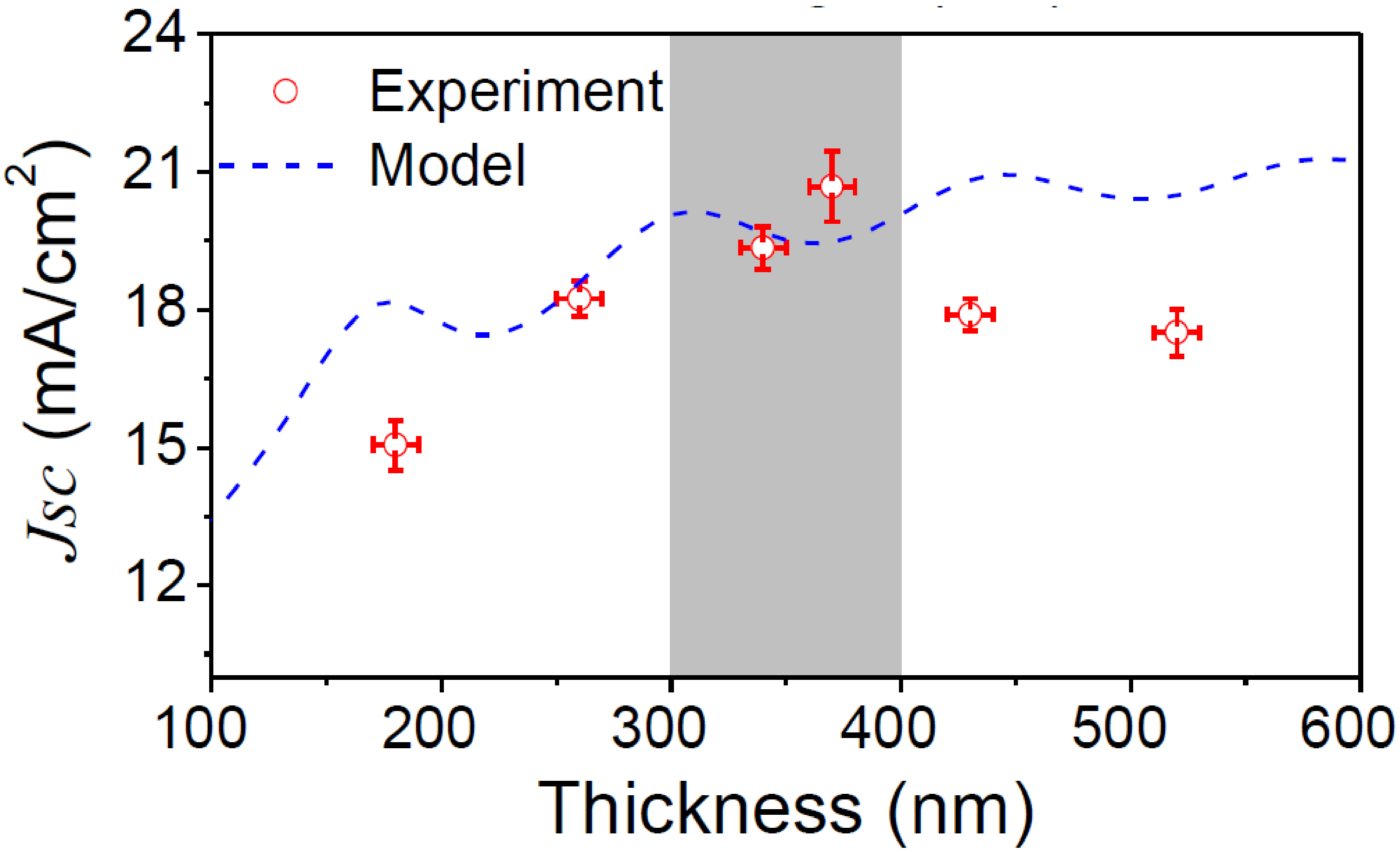
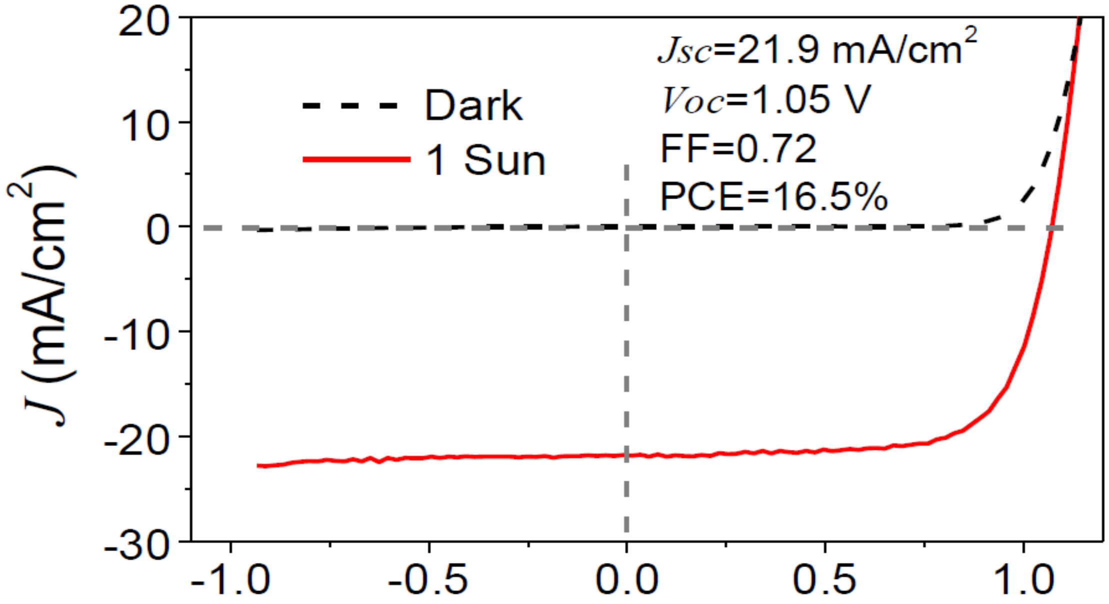
Experiment versus Model



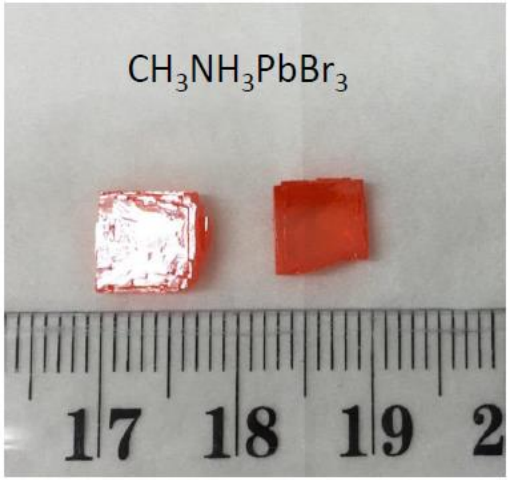
The Optimised Outcome

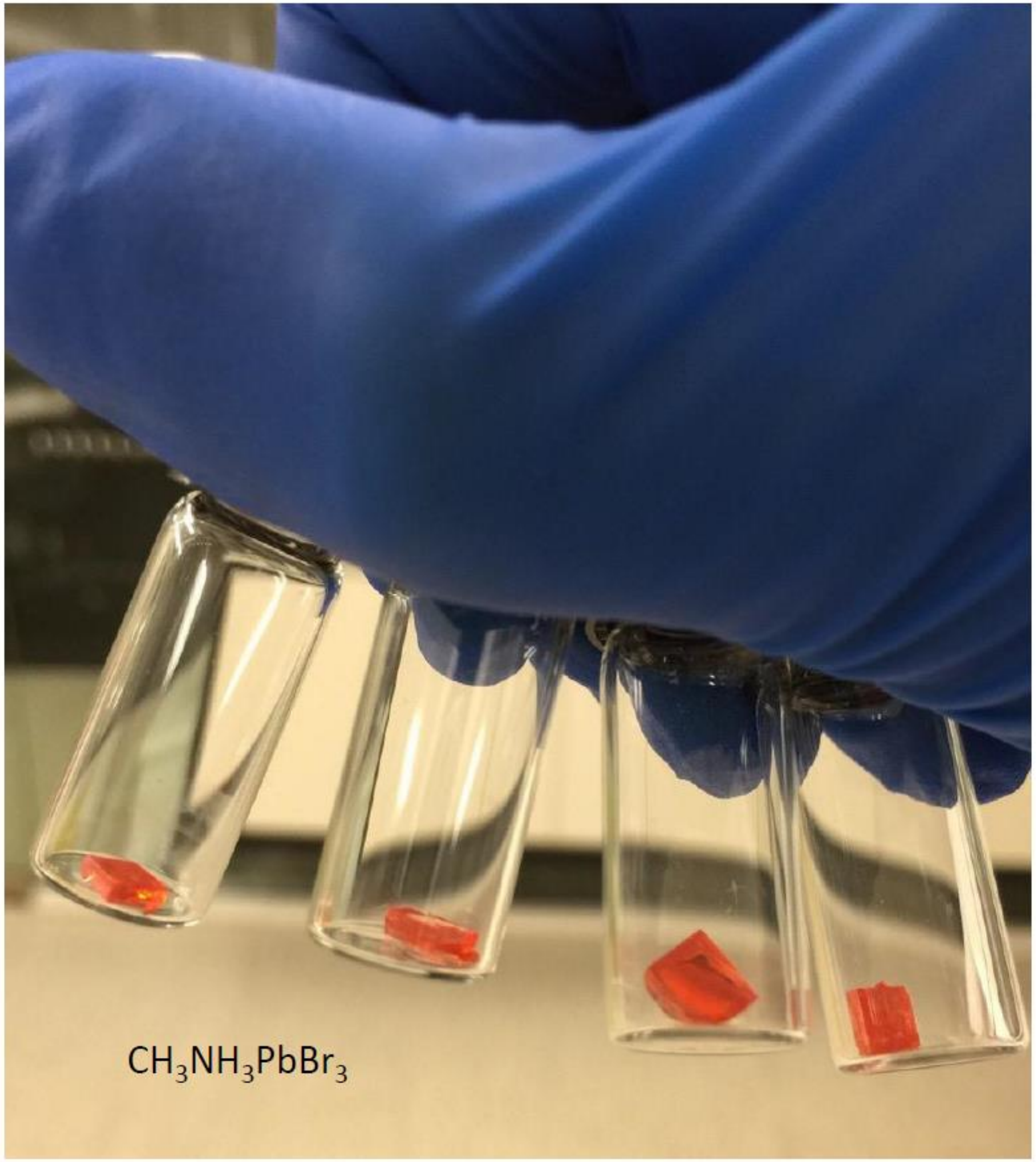
Glass/ITO (80 nm)/PEDOT:PSS (15 nm)/ PCDTBT (5 nm)/Junction (370 nm)/PC60BM (10 nm) /Ag (100 nm)



	J_{sc} (mA/cm^2)	V_{oc} (V)	FF	PCE (%)
180 nm	15.1±0.6	1.05±0.00	0.74±0.06	11.2±0.7
260 nm	18.2±0.4	1.04±0.01	0.69±0.03	13.1±0.6
340 nm	19.4±0.5	1.05±0.01	0.73±0.02	14.6±0.4
370 nm	20.7±0.8	1.05±0.01	0.71±0.02	15.2±1.1
430 nm	17.9±0.4	1.05±0.01	0.73±0.03	13.7±0.4
520 nm	17.5±0.5	1.03±0.01	0.61±0.04	10.9±1.1

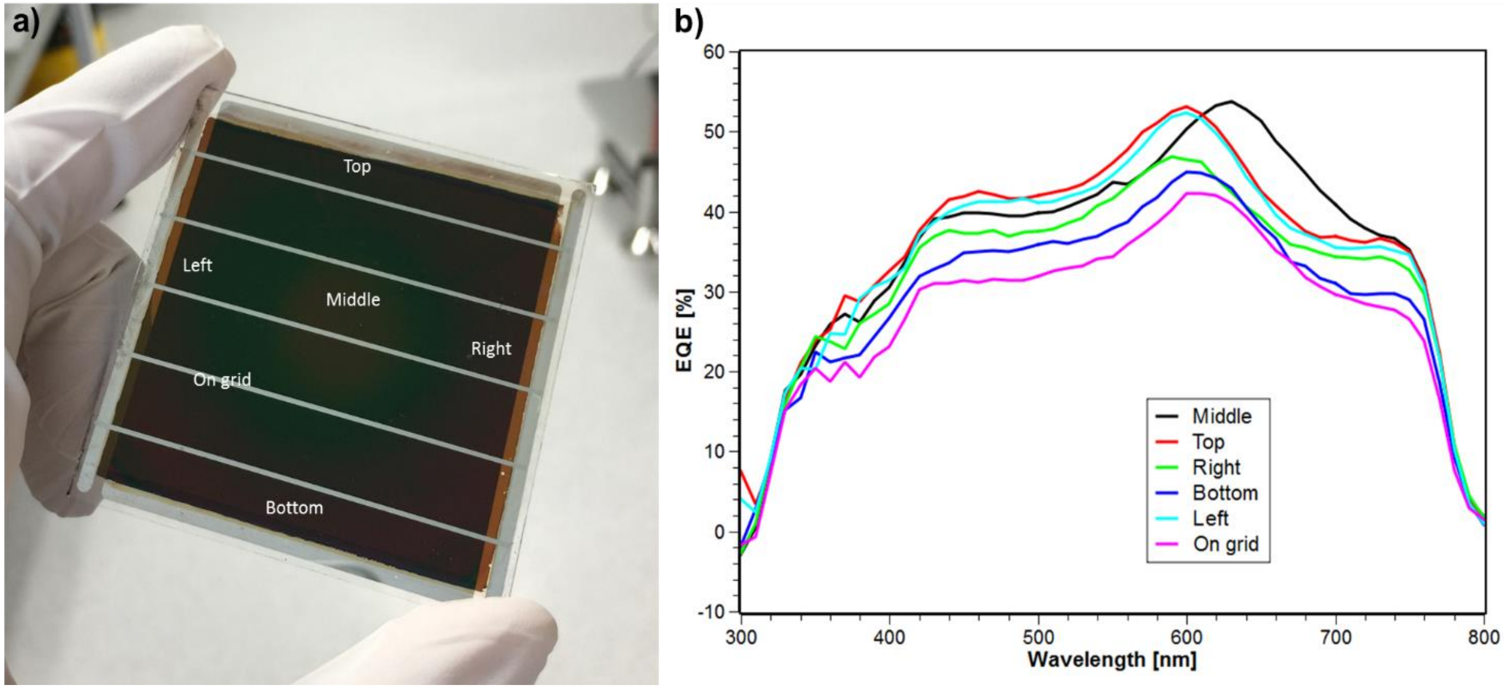
Hysteresis Free & V_{oc} dependent upon electrode work function offset





What next? Vincent’s sugar cubes.

Scaling ……


a)
Top
Left
Middle
Right
On grid
Bottom
b)
EQE [%]
60
50
40
30
20
10
0
-10
300
400
500
600
700
800
Wavelength [nm]
Middle
Top
Right
Bottom
Left
On grid

A Culture Changing Project: The UQ MW Array

(http://www.uq.edu.au/solarenergy/index.html)

Key Statistics:

-9.3 GW hr in 56 months;

-17.8% Capacity Factor;

-8.9MKg of CO_2 mitigated;

- > 1500 visitors;

-~ $1.2M in savings;

-On-track for 8-10 year payback;

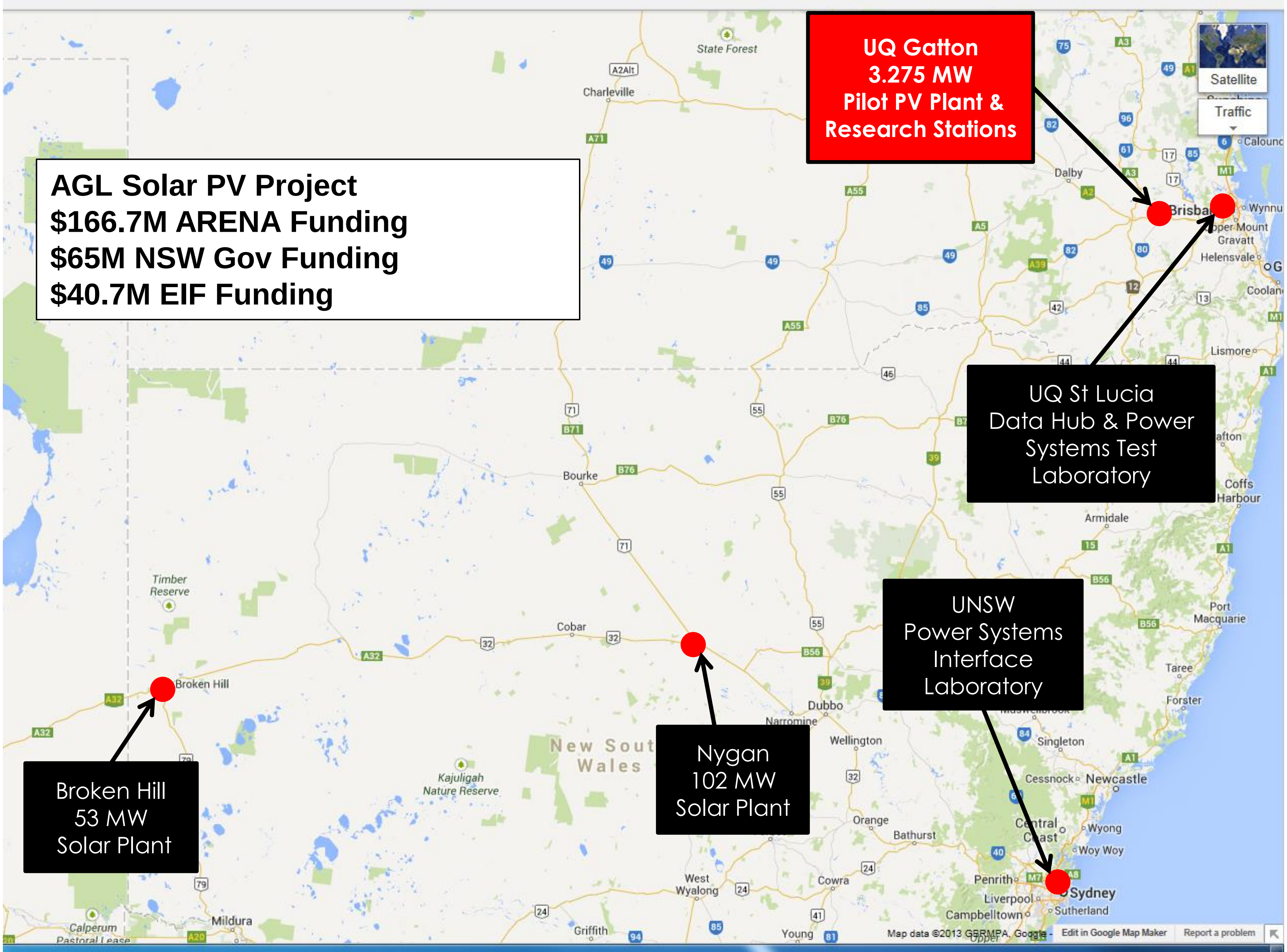
-Big research potential;

-Data being used by industry, government and research organisations;

-Still the largest roof-top PV system in AU!

SYSTEMS THINKING

AGL SOLAR PV PROJECT



AGL Solar PV Project
$166.7M ARENA Funding
$65M NSW Gov Funding
$40.7M EIF Funding

UQ Gatton
3.275 MW
Pilot PV Plant &
Research Stations

UQ St Lucia
Data Hub & Power
Systems Test
Laboratory

UNSW
Power Systems
Interface
Laboratory

Nygan
102 MW
Solar Plant

Broken Hill
53 MW
Solar Plant

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

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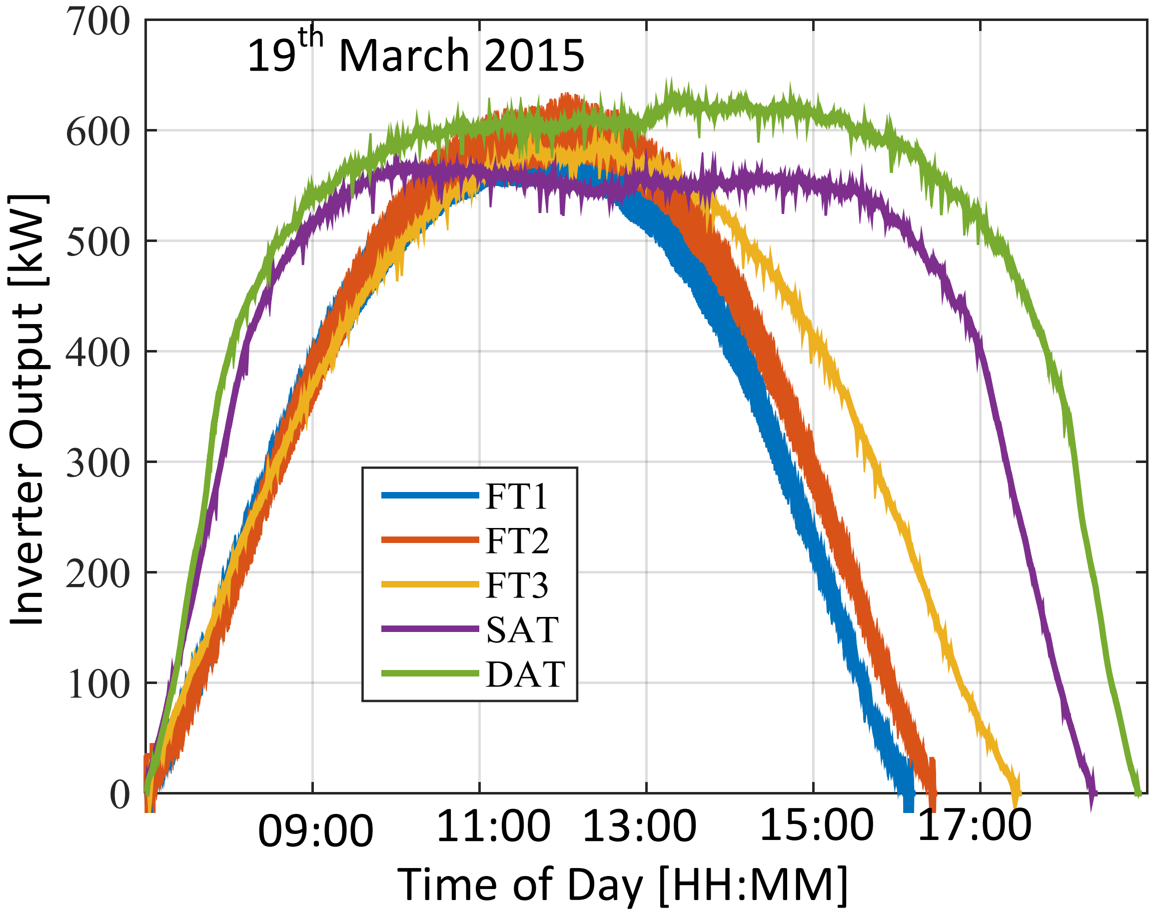
http://solar-energy.uq.edu.au/

PV Array Performance

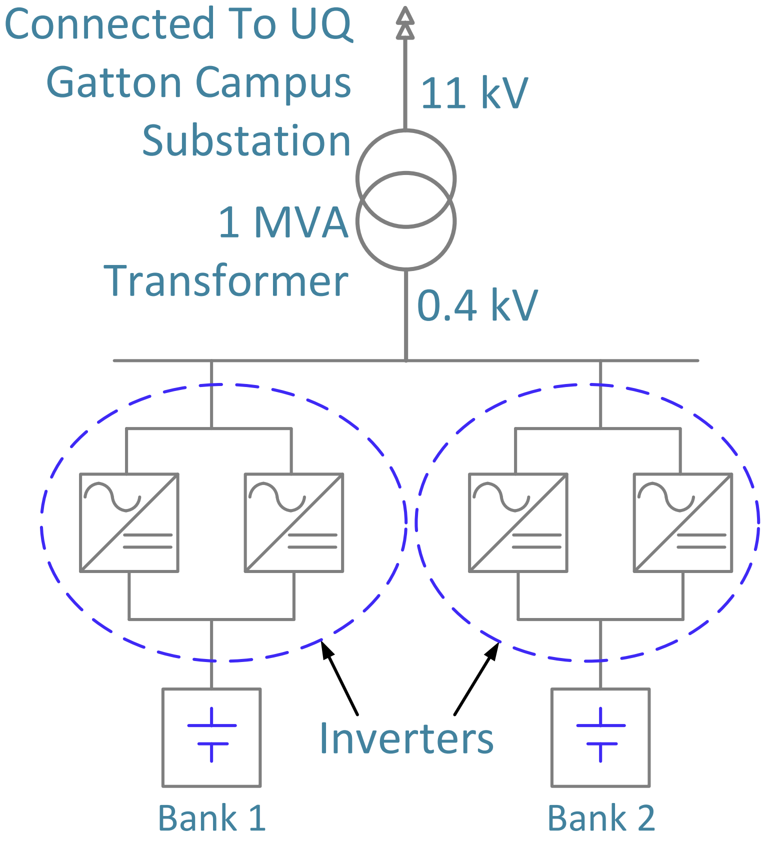


Array Energy (MWh):

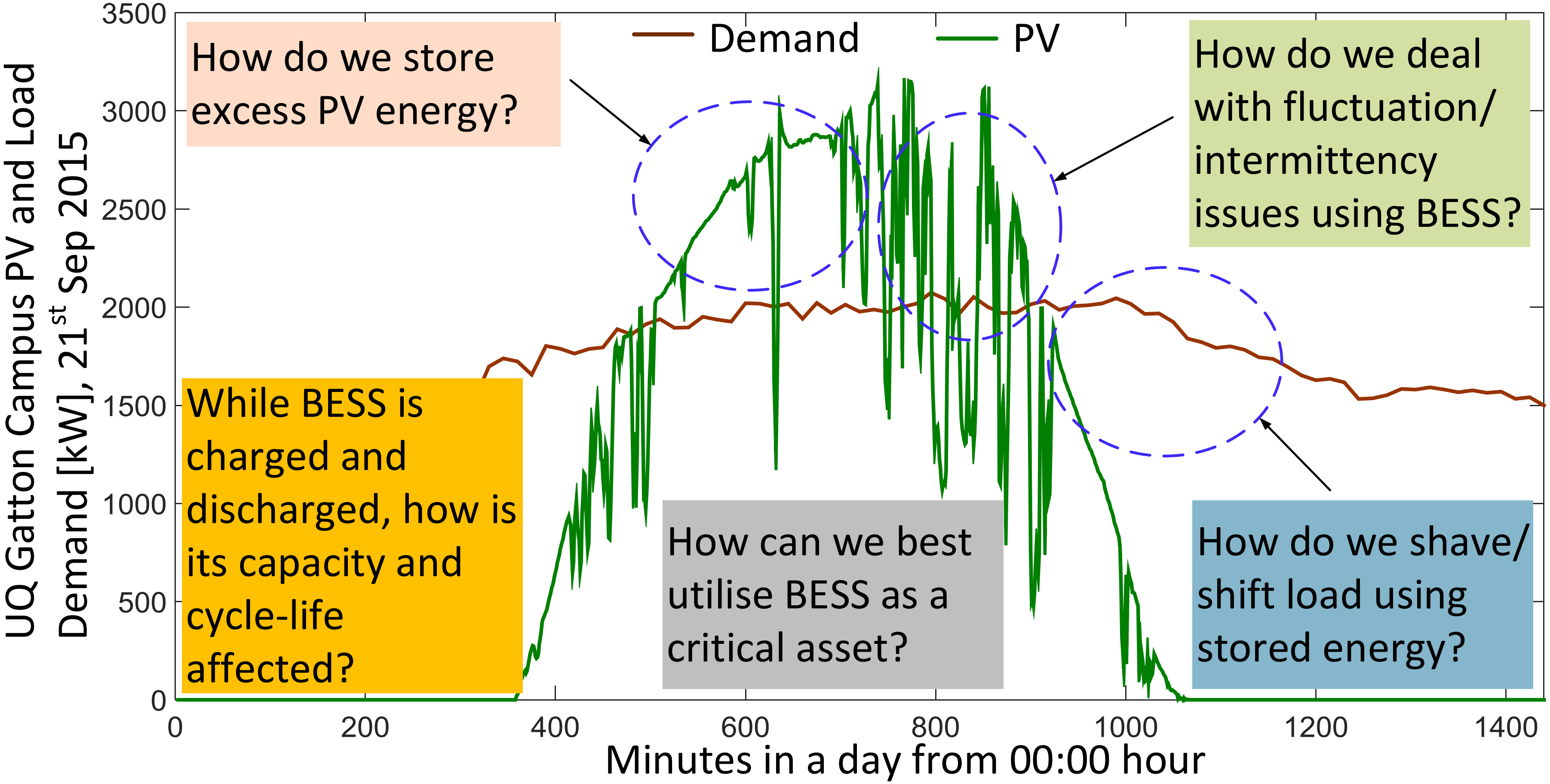
- FT1: 4.27
- FT2: 4.40
- FT3: 4.25
- SAT: 4.82
- DAT: 5.19
- Total = 22.93 MWh (30.3% CF)

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?

How do we deal with fluctuation/ intermittency issues using BESS?

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

How can we best utilise BESS as a critical asset?

How do we shave/ shift load using stored energy?

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

Queensland Government

gciQ Global Change Institute

ACAP

Australian Government
Australian Research Council

ARENA

The University Of Queensland
AUSTRALIA

UQ SOLAR
Australia's largest flat-panel photovoltaic installation is here.

Exciton binding energy – low frequency or optical ε'?

Solution to the Wannier (Mott) equation:

$$E_B = \frac{\mu}{m_0}\frac{1}{\epsilon^2}\frac{m_0 e^4}{2(4\pi\epsilon_0\hbar)^2}$$

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 $CH_3NH_3PbI_3$ exciton separation >> lattice constant and static ε must be used.

$$\frac{4\,\pi^2\hbar^4\epsilon^2\epsilon_0^2}{\mu^3 e^2} = c_0$$

[Roth et al. *Phys. Rev*. **114**, 90-103 (1959)]

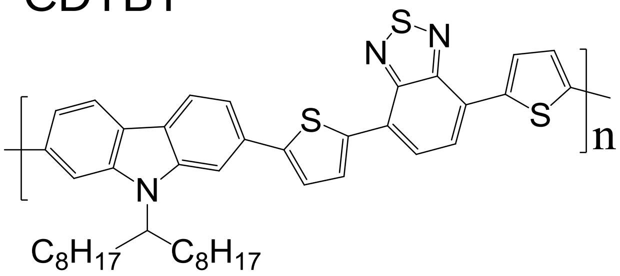
$c_0 \sim 1.35 \text{ x } 10^{-6}\ \mathrm{eV/T^2}$ to $2.7 \text{ x } 10^{-6}\ \mathrm{eV/T^2}$ [Tanaka et al. *Solid State Commun*. **127**, 619-623 (2003)]

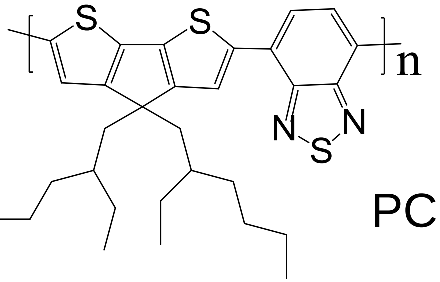
$$\boxed{1.7\ meV < E_B < 2.1\ meV}$$

[D'Innocenzo et al. *Nature Commun*. **5**, 3586 (2014): ~ 50 meV]
[Frost et al. *Nano Lett*. **14**, 2584-2590 (2014): < 1meV]

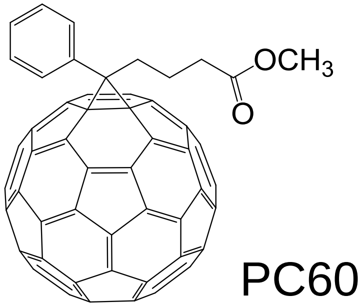
n-and-*p*-type electrode interlayers

PCDTBT

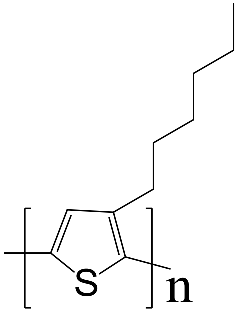




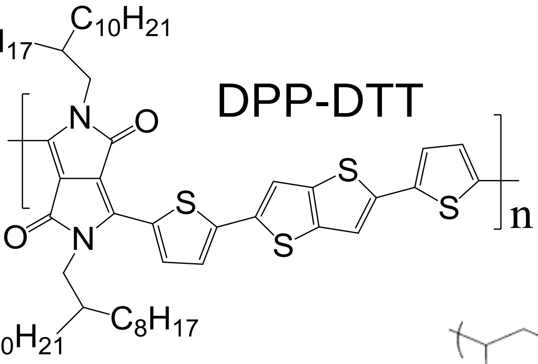
PCPDTBT



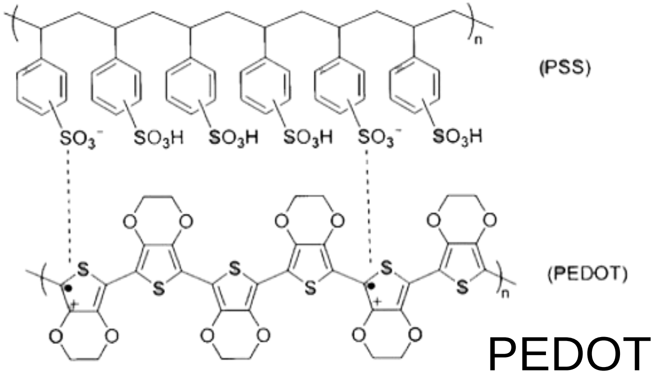
PC60BM



P3HT

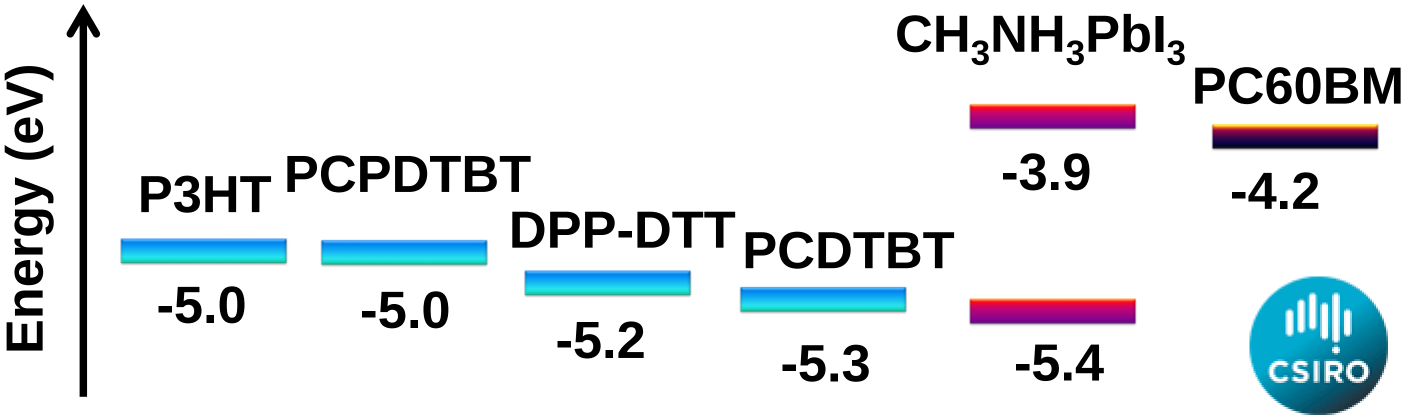


DPP-DTT



PEDOT:PSS

Electrode interlayers



Energy (eV)

P3HT
-5.0

PCPDTBT
-5.0

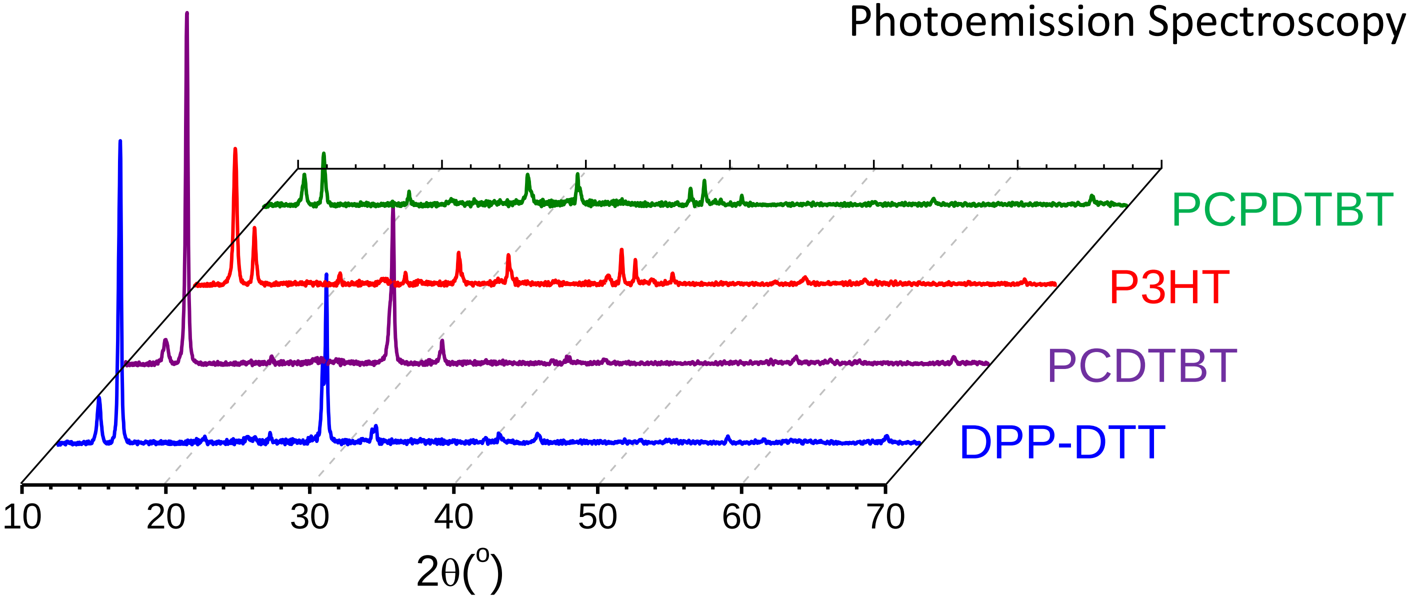
DPP-DTT
-5.2

PCDTBT
-5.3

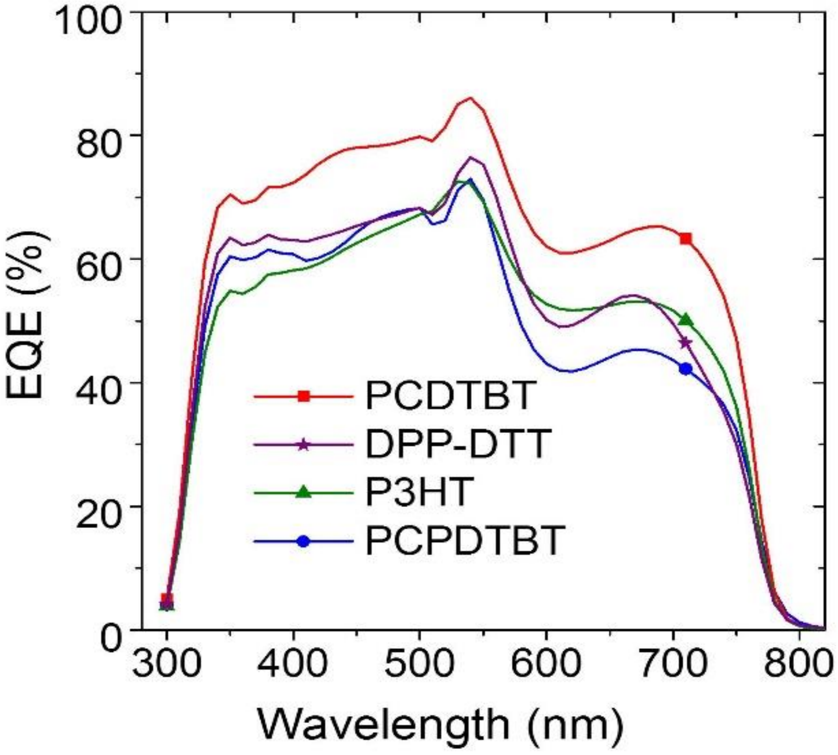
$CH_3NH_3PbI_3$
-3.9
-5.4

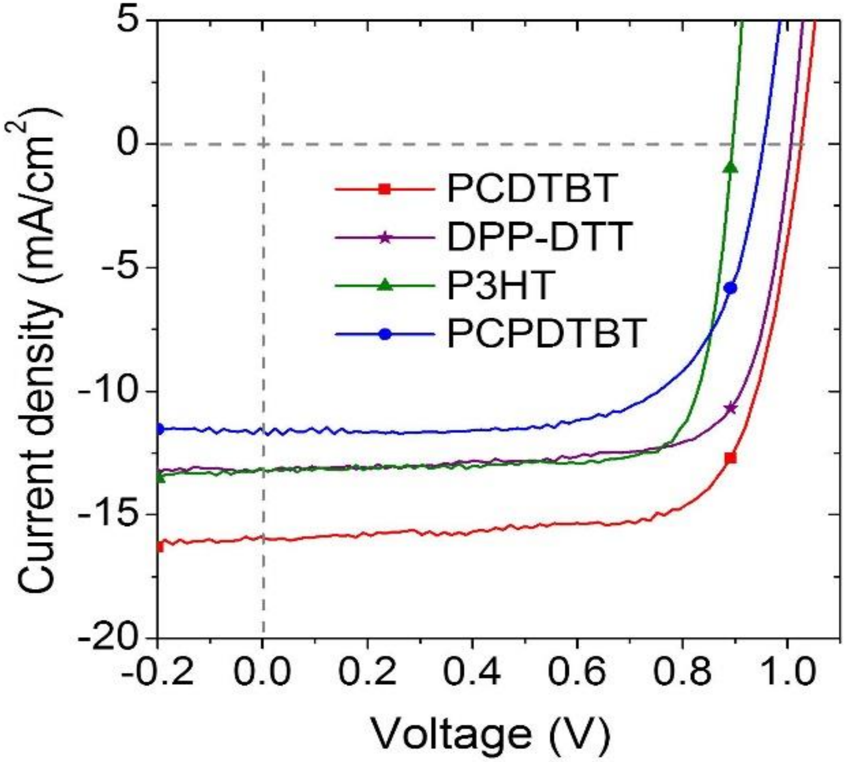
PC60BM
-4.2

Photoemission Spectroscopy in Air



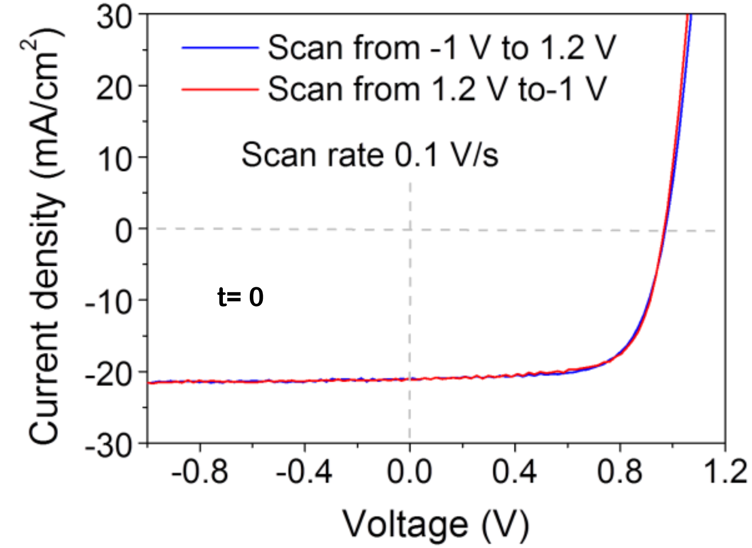
3. Electrode work function difference influences V_{oc}

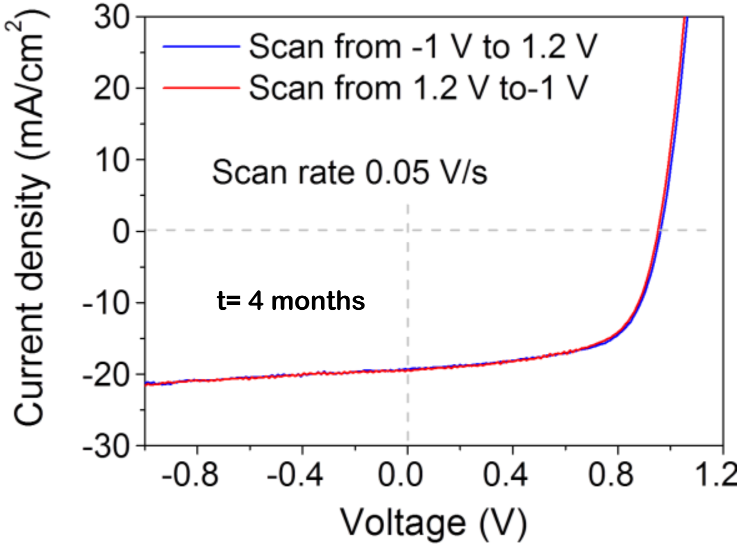


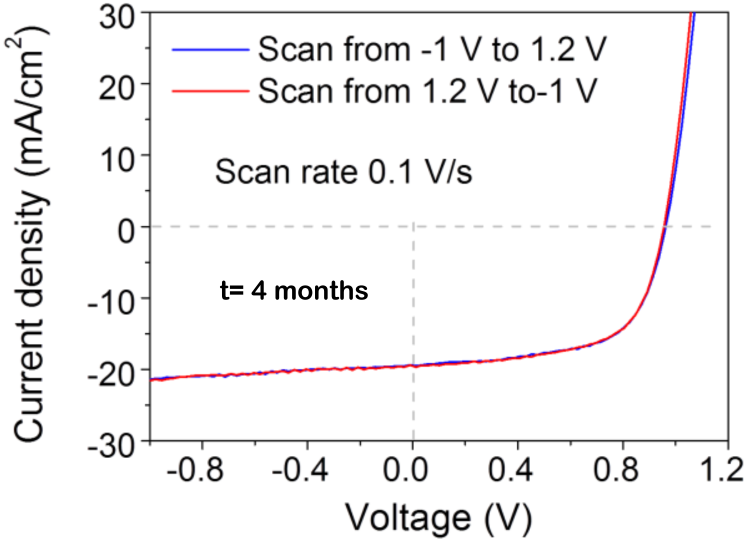


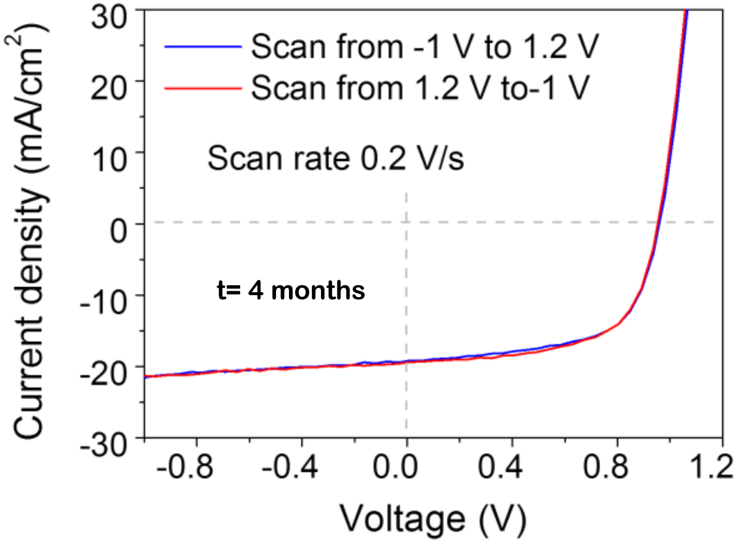
	J_{sc} (mA/cm^2)	V_{oc} (V)	FF	PCE (%)
PCDTBT	15.9±0.7	1.03.±0.01	0.66±0.05	10.9±0.8
DPP-DTT*	13.3	1.00	0.74	9.8
P3HT	14.2±0.9	0.70±0.10	0.78±0.03	8.5±0.8
PCPDTBT	13.0±0.8	0.88±0.06	0.69±0.04	7.8±0.8

Hysteresis: interfacial phenomenon?









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!