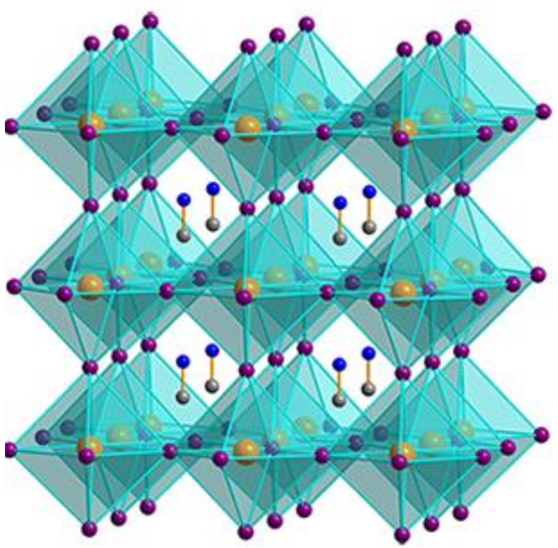
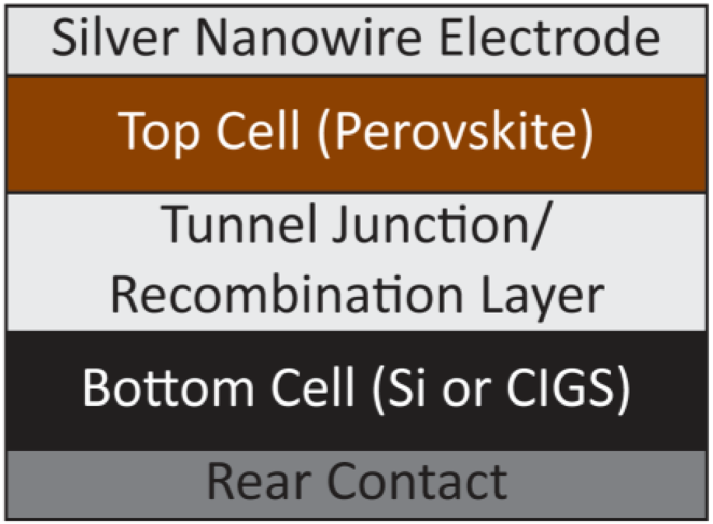
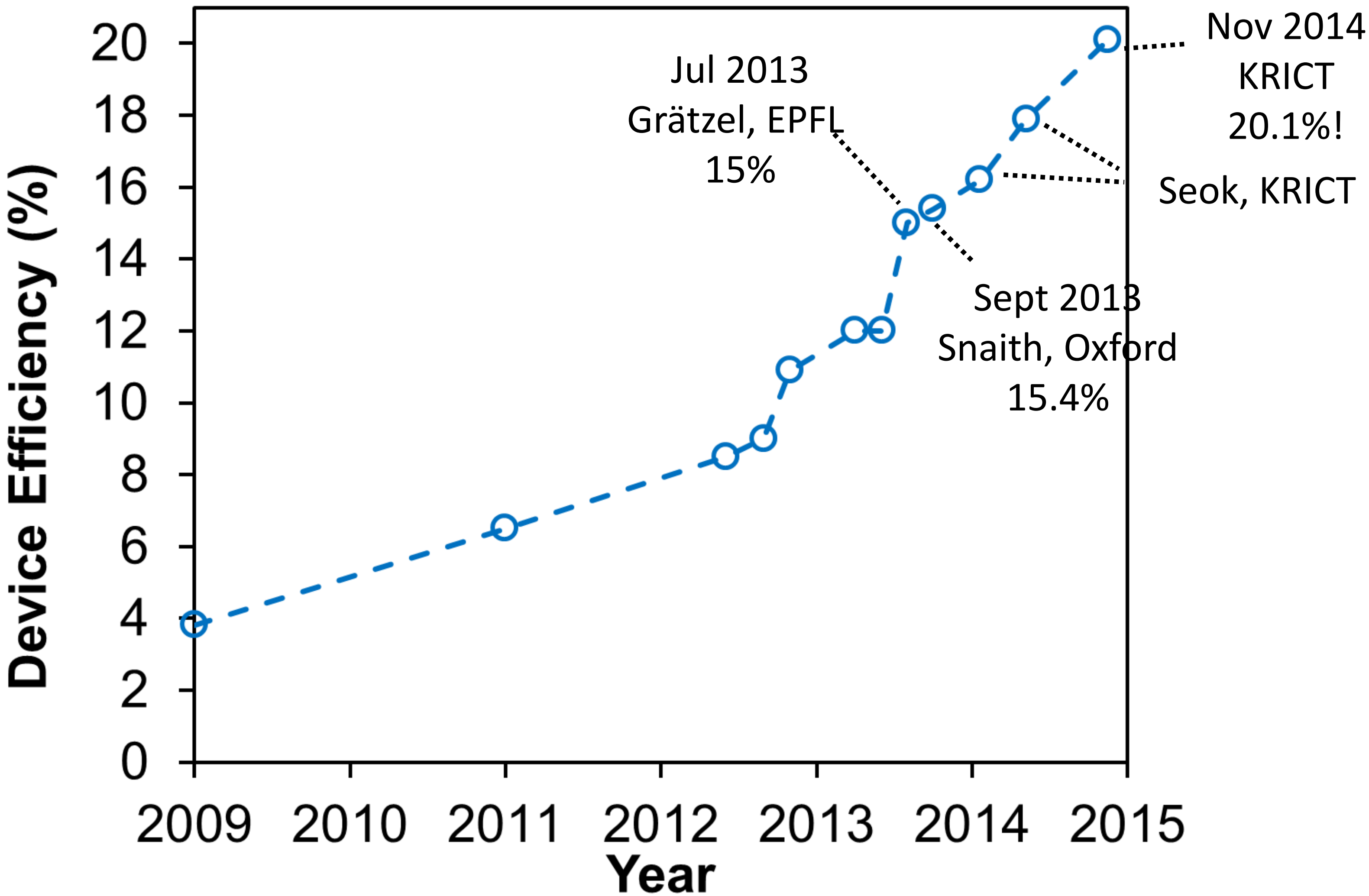
Novel Inorganic-Organic Perovskites for Solution Processed Photovoltaics

PIs: Mike McGehee and Hema Karunadasa





Perovskite Solar Cells are Soaring



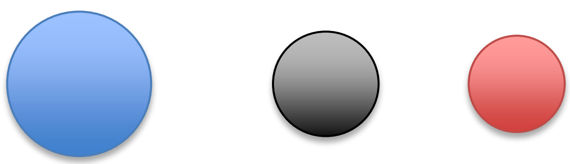
Grätzel et al., *Nature* 2013; Snaith et al., *Nature* 2013; Seok et al. *Nature Materials* 2014; Seok et al. *Nature* 2015

Perovskites

Generic formula: ABX_3 , where X = oxygen or halide

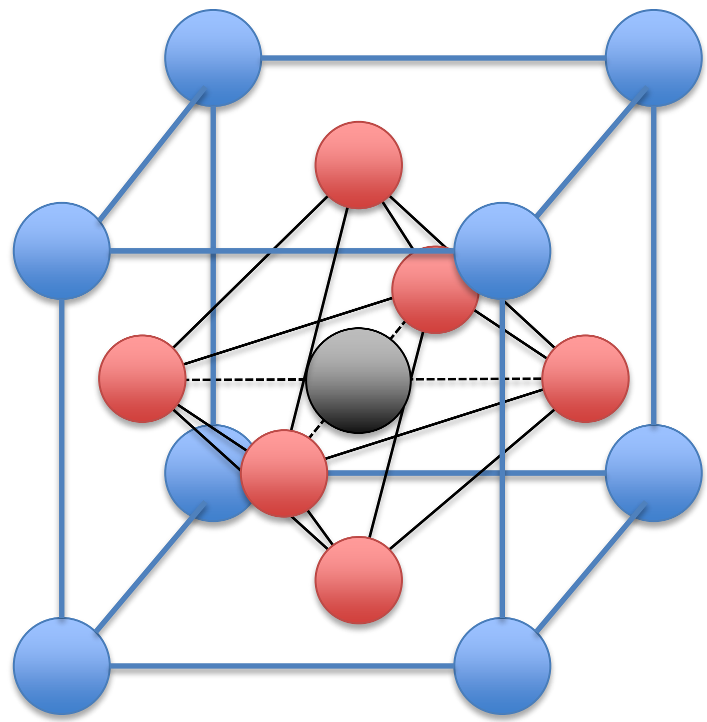
A cation 12-fold, B-cation 6-fold co-ordinated with X anion

$CH_3NH_3^+$ Pb^{2+} I^-



$CH_3NH_3PbI_3$

Methylammonium-lead-iodide



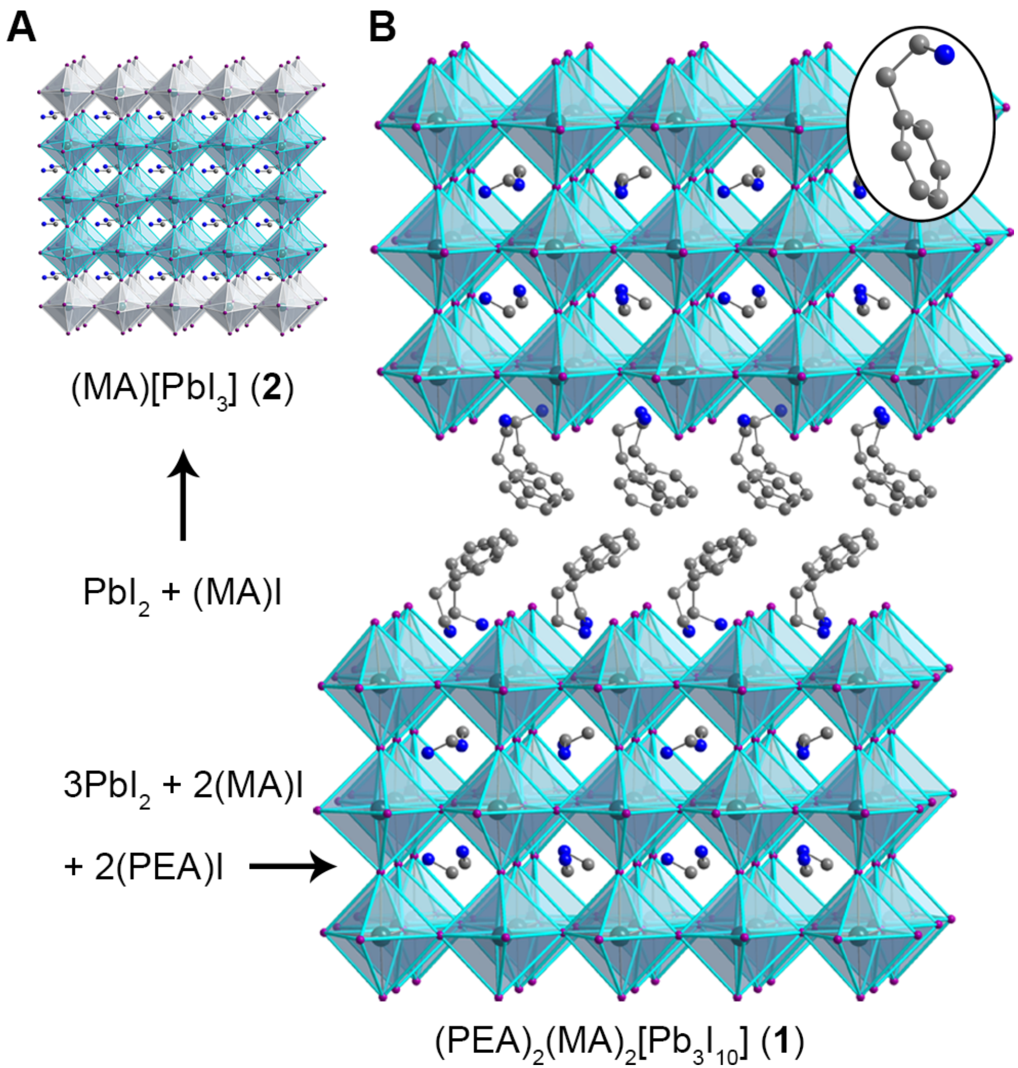
What we know about perovskites

- Solution deposition or evaporation can be used
- Absorbs light better than GaAs
- Charge carrier mobility around 10-30 cm^2/Vs
- $E_g - qV_{OC}$ can be as small as 0.38 V
- Carrier lifetimes > 1 μs even in polycrystalline films
- Very little surface recombination

- Ions move around, screening the electric field and causing hysteresis
- Methyl ammonium leaves the film at T as low as 80˚C
- Having an impermeable electrode is essential

- Device modeling talk tomorrow by Becky Belisle

A 2D perovskite solar-cell absorber with enhanced moisture resistance

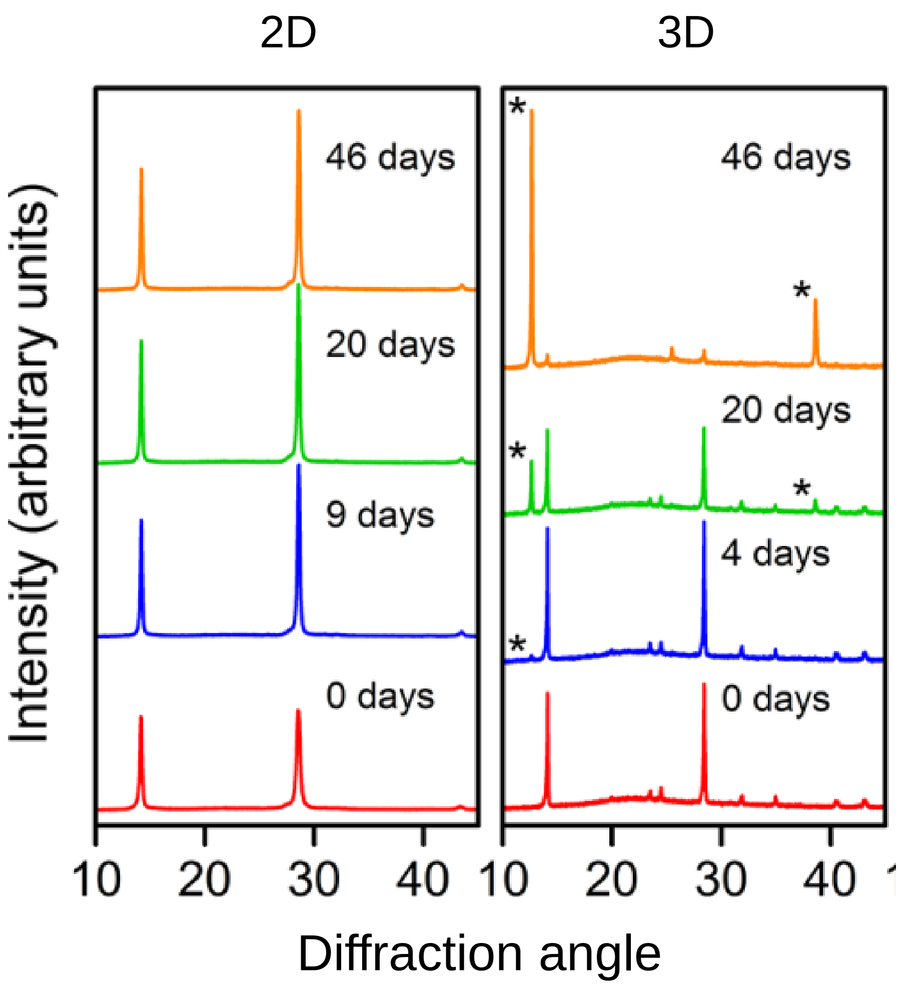


<u>Advantages of the 2D structure</u>

- The larger bandgap affords a higher open-circuit voltage of 1.18 V
- High-quality films can be deposited through one-step spin-coating and annealing is not required

Smith, Hoke, Solis-Ibarra, McGehee and Karunadasa *Angew. Chem., Int. Ed.* **2014,** *53*, 11232

A 2D perovskite solar-cell absorber with enhanced moisture resistance



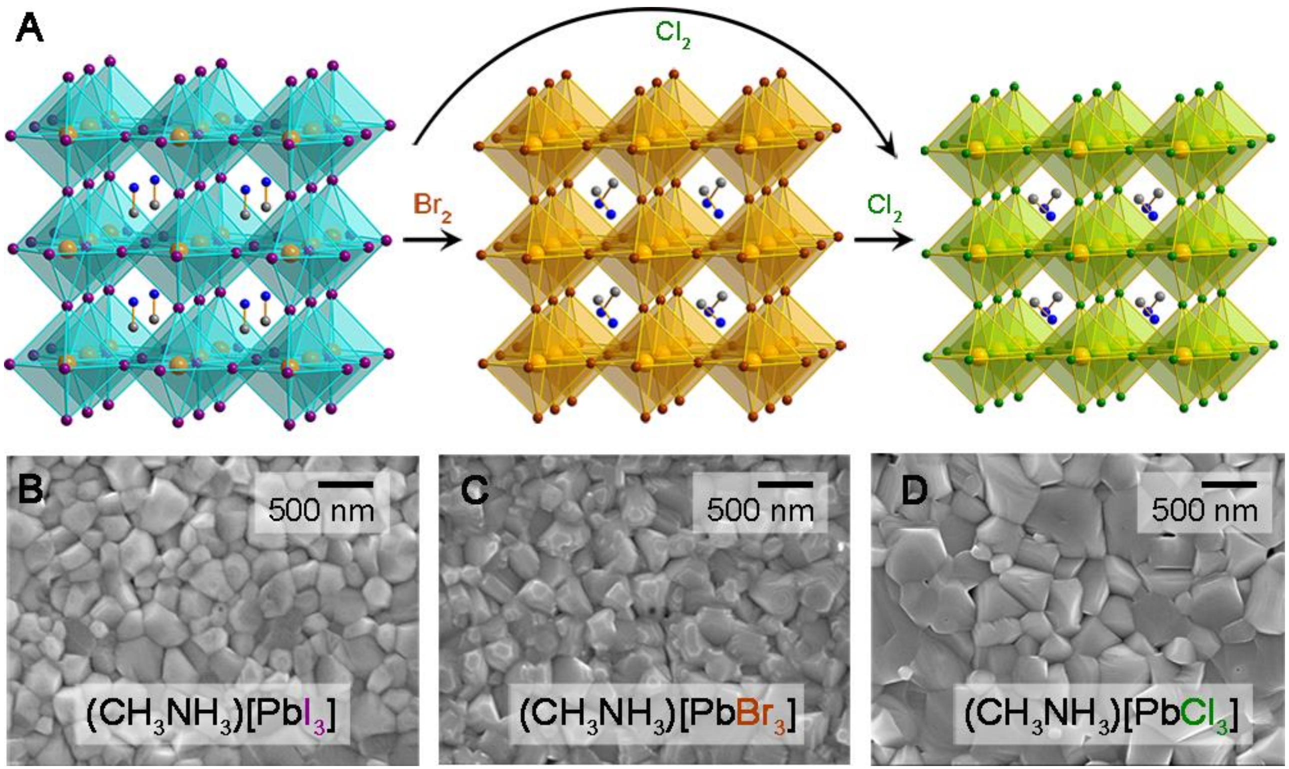
At 55% relative humidity. * Denotes reflections from PbI_2

Advantages of the 2D structure

- The larger bandgap affords a higher open-circuit voltage of 1.18 V
- High-quality films can be deposited through one-step spin-coating and annealing is not required
- The material is far more moisture resistant and devices can be fabricated under humid atmospheres

Smith, Hoke, Solis-Ibarra, McGehee and Karunadasa *Angew. Chem., Int. Ed.* **2014,** *53*, 11232

Post-synthetic halide conversion in 3D perovskites



- Many methods have been developed for obtaining the continuous Pb−I films required for optoelectronic devices. But similar processing does not form high-quality Pb−Br or Pb−Cl films
- Exposing Pb−I films to Br_2 or Cl_2 vapor forms high-quality Pb−X (X = Br or Cl) films with no purification or annealing steps required

Solis-Ibarra, Smith and Karunadasa, *Chem. Sci.* **2015,** *6*, 4054

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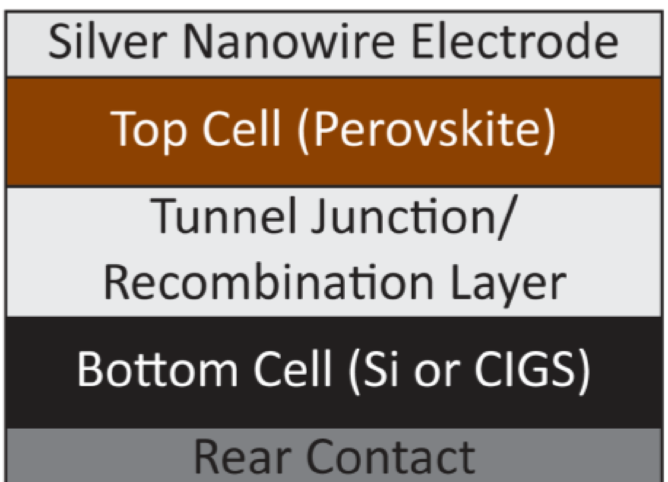
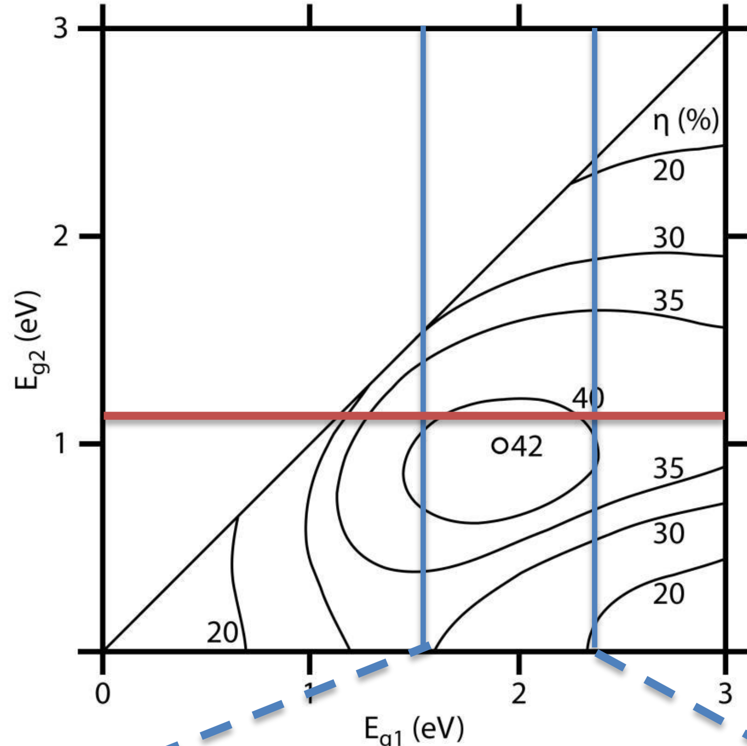
Perovskites in Polycrystalline Tandems

Colin Bailie, Greyson Christoforo, Jonathan Mailoa, Andrea Bowring, Eva Unger, William Nguyen, Erik Hoke, Julian Burschka, Norman Pellet, Jungwoo Lee, Alberto Salleo, Rommel Noufi, Michael Grätzel, Tonio Buonassisi, Michael McGehee



Use Double Junction Tandems to Reach >30% Efficiency



A. De Vos, ***J. Phys. D. Appl. Phys.***, 1980, **13** 839-846

1.1eV Si or CIGS

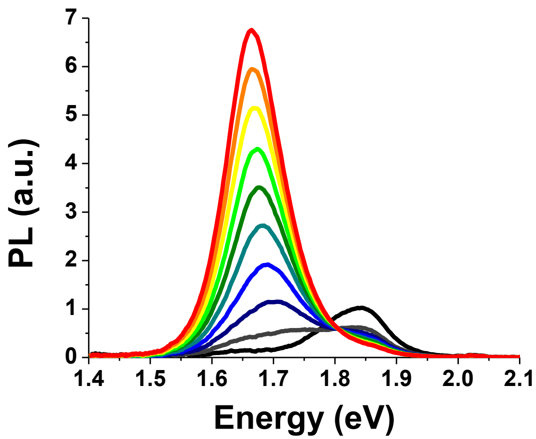
$CH_3NH_3PbI_3$
E_g=1.6 eV

$(MA)Pb(Br_xI_{1-x})_3$

$CH_3NH_3PbBr_3$
E_g=2.3 eV

Mixed halides with high band gaps are unstable

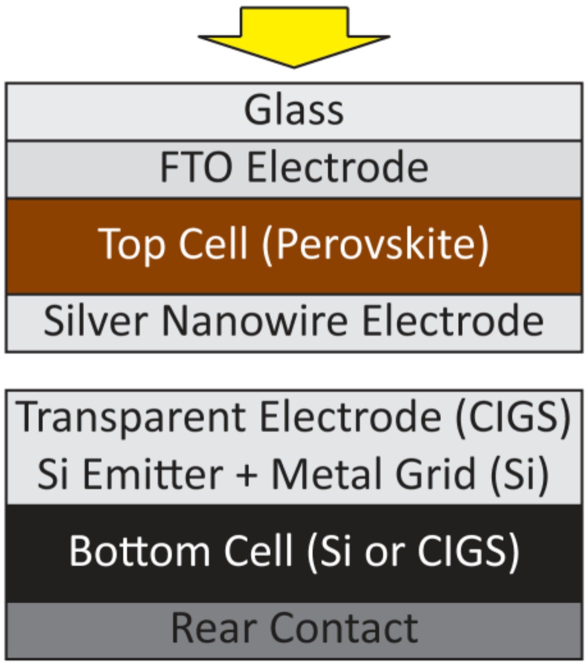
- $CH_3NH_3Pb(Br_xI_{1-x})_3$ ($0.2<x\leq0.9$) undergoes reversible halide segregation under illumination forming iodide enriched (x~0.2) minority phase.



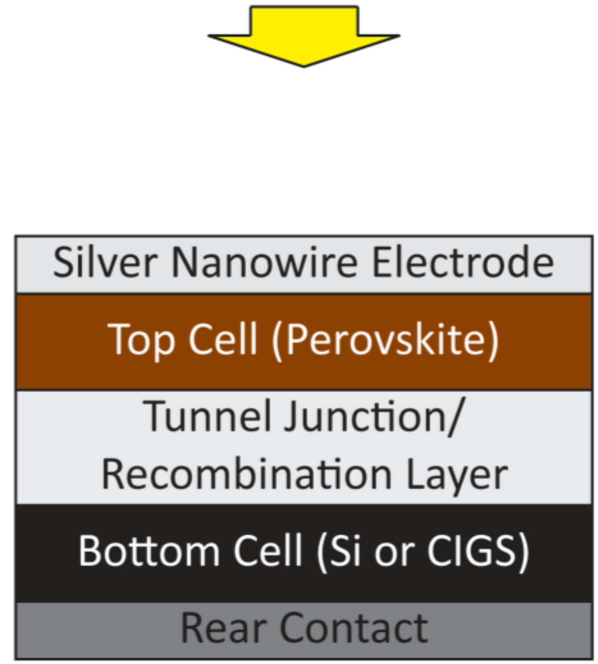
- A more stable high band gap perovskite is needed.

E. T. Hoke, M. M. McGehee, et al., ***Chem. Sci.***, 2014 **6** 613-617

Hybrid Tandem Architectures



Mechanically-stacked
- Easier prototyping
- No current matching required
- No tunnel junction or recombination layer required



Monolithically-integrated
- Fewer layers that parasitically absorb
- Module fabrication easier

C. D. Bailie, M. G. Christoforo, M. D. McGehee, et al., ***Energy Environ. Sci.,*** 2015, **8** 956-963.
C. D. Bailie, M. D. McGehee MRS Bulletin, 40 (2015) 681-5.

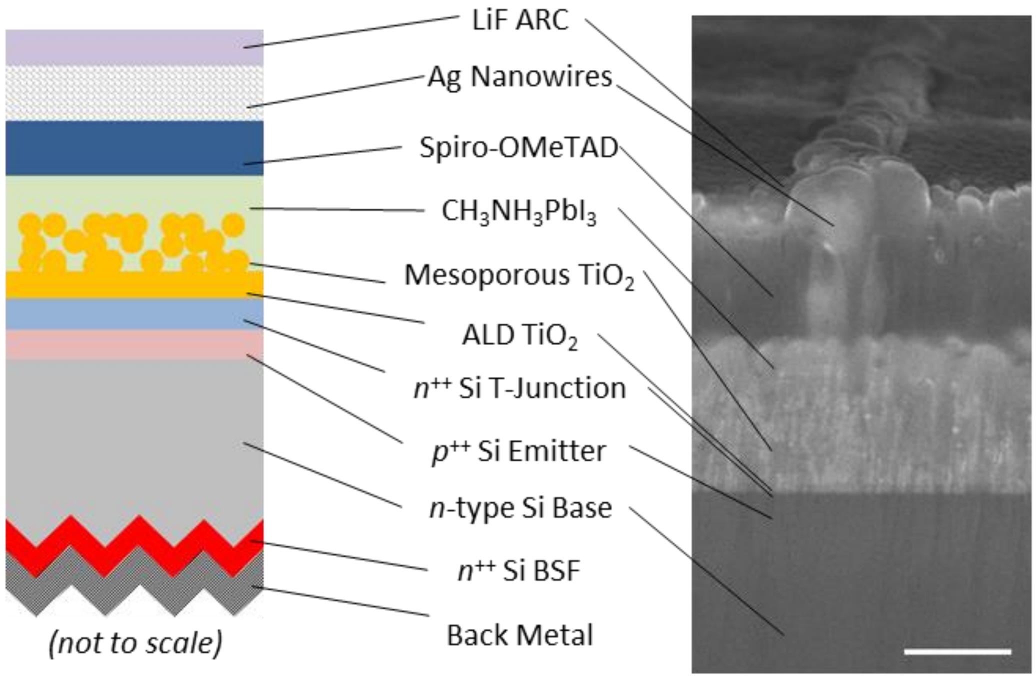
4-Terminal Tandem of Perovskite on CIGS Provides Net Benefit

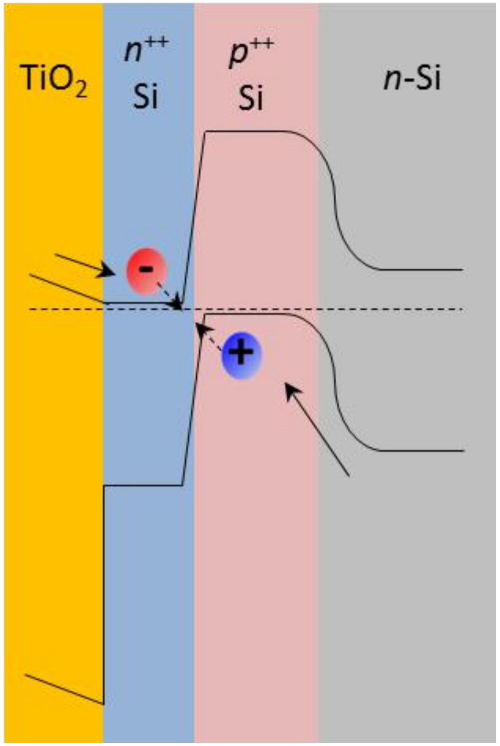
Cell	Jsc (mA/cm^2)	Voc (mV)	FF (-)	Efficiency (%)
Perovskite	17.5	1025	0.710	12.7
CIGS	31.2	711	0.768	17.0
Filtered CIGS	10.9	682	0.788	5.9
4-Terminal Tandem	**-**	**-**	**-**	**18.6**

CIGS from Rommel Noufi (NREL)

C. D. Bailie, M. G. Christoforo, M. M. McGehee, et al., ***Energy Environ. Sci.,*** 2015, **8** 956-963

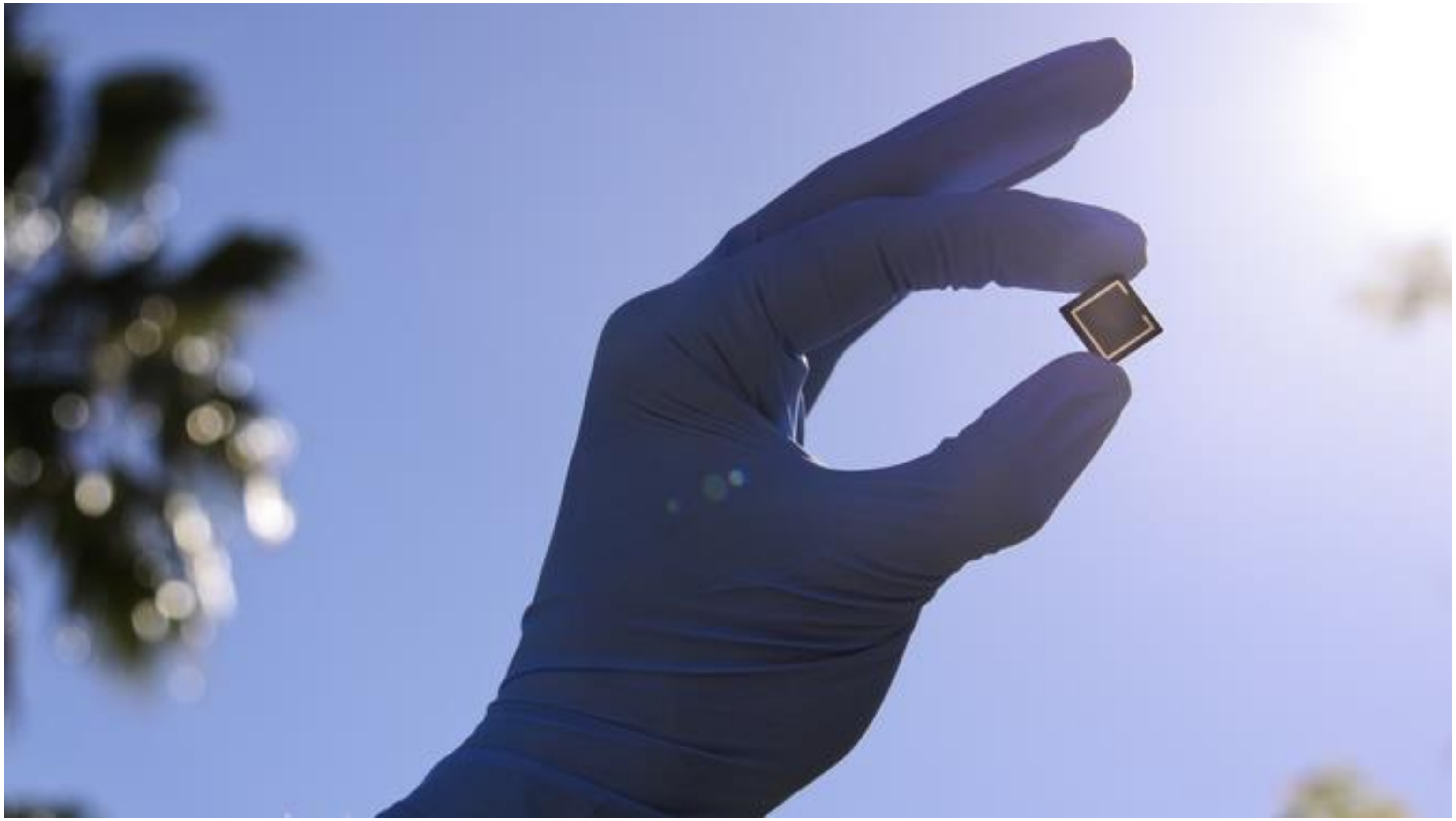
Monolithic integration of the perovskite cell onto a silicon wafer





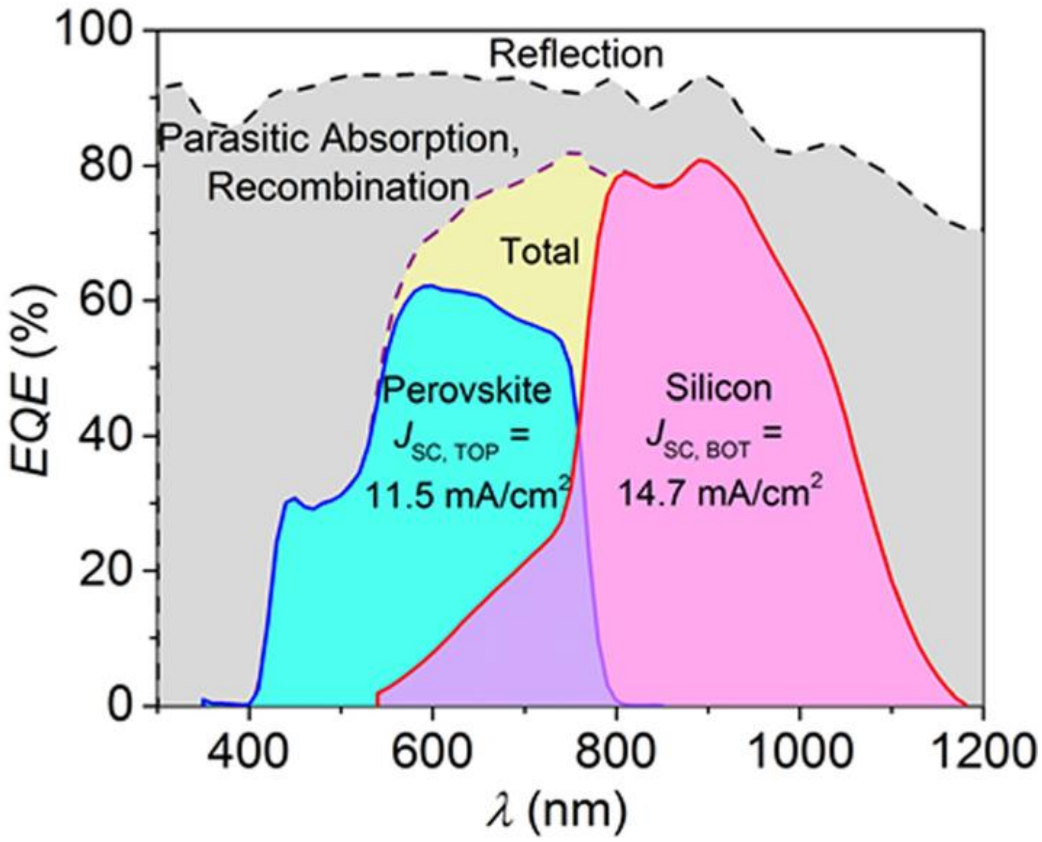
J.P. Mailoa, C. D. Bailie, M. M. McGehee, T. Buonassisi, et al., ***Appl. Phys. Lett.,*** 2015, **106** 121105

1 cm^2 monolithic tandem



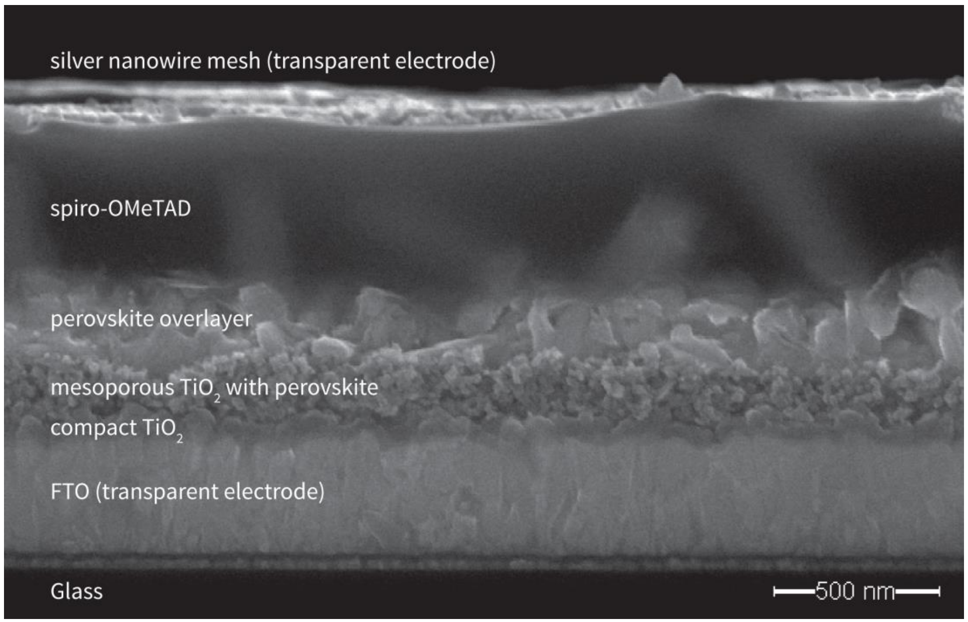
13.7 % efficiency

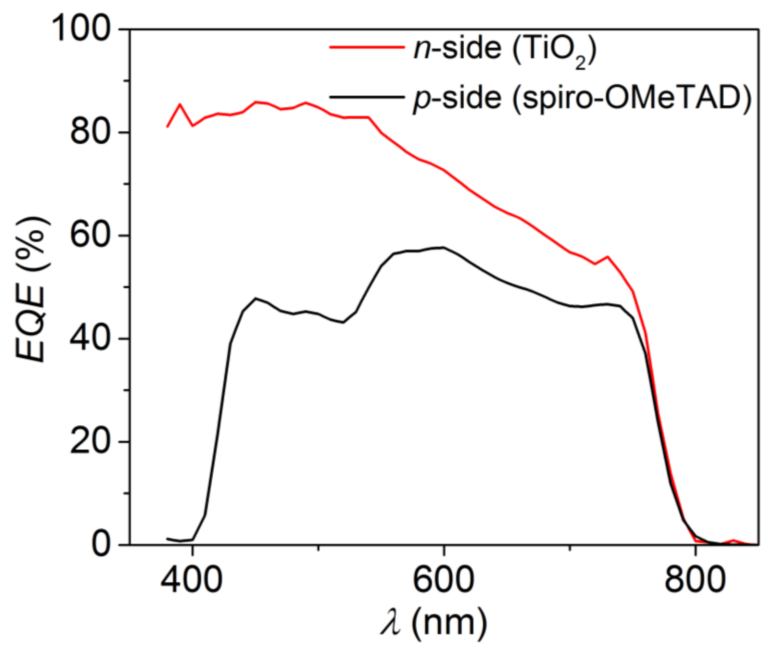
Tandem is current-limited by the perovskite sub-cell



J.P. Mailoa, C. D. Bailie, M. M. McGehee, T. Buonassisi, et al., ***Appl. Phys. Lett.,*** 2015, **106** 121105

Illumination direction of a semi-transparent perovskite cell is important

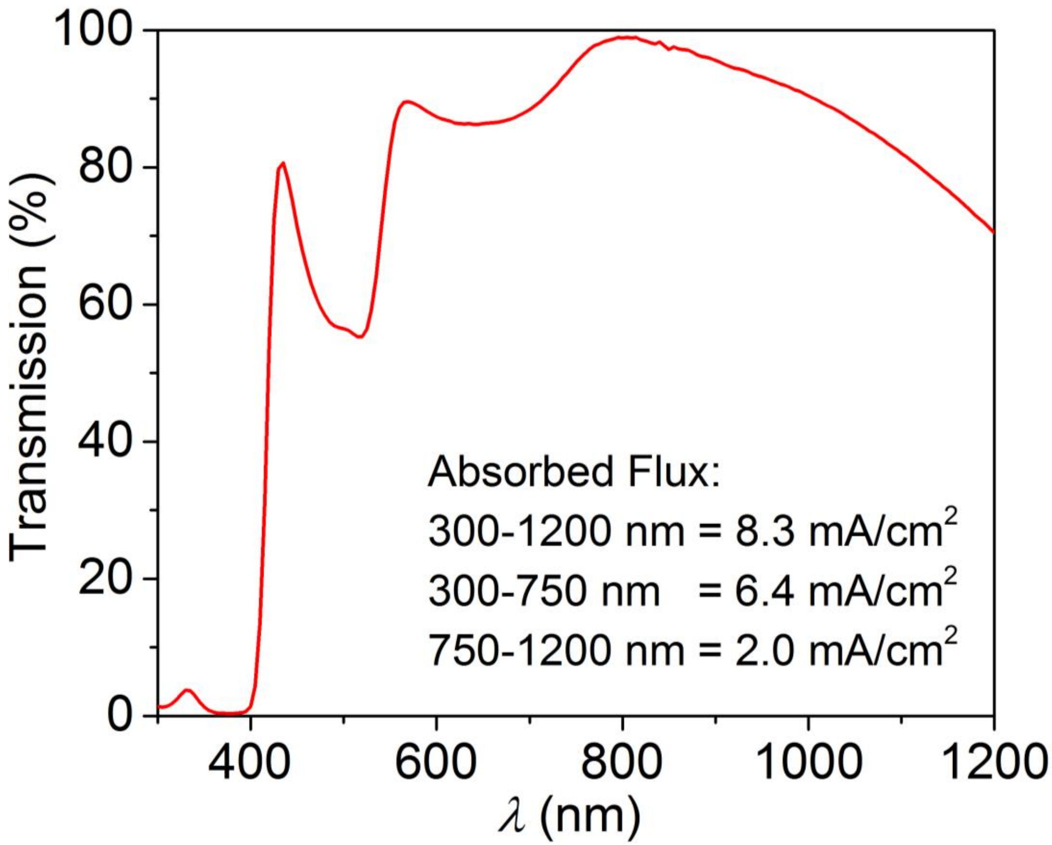




n-side (TiO2) illumination integrates to 17.3 mA/cm^2 while *p*-side illumination (spiro-OMeTAD) integrates to 11.4 mA/cm^2

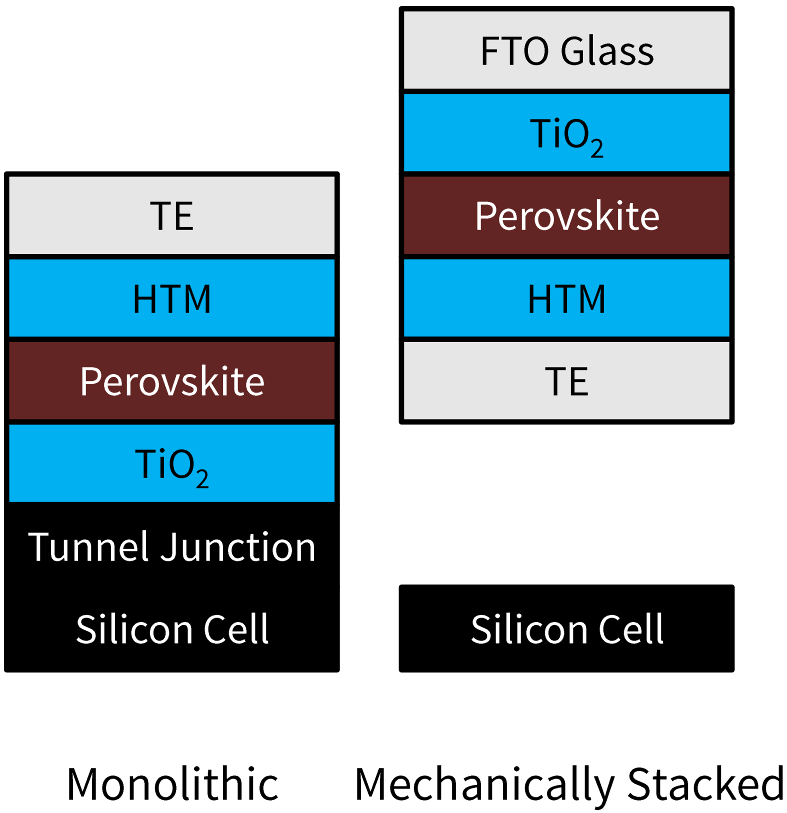
J.P. Mailoa, C. D. Bailie, M. M. McGehee, T. Buonassisi, et al., ***Appl. Phys. Lett.,*** 2015, **106** 121105

Parasitic absorption from spiro-OMeTAD limits the photocurrent



J.P. Mailoa, C. D. Bailie, M. M. McGehee, T. Buonassisi, et al., ***Appl. Phys. Lett.,*** 2015, **106** 121105

Opportunities for Improvement



Transparent electrode + barrier film:
- prevent halogen corrosion of electrode
- deposition does not damage active layers

Parasitic absorption in heterojunctions:
- thinner and less absorbing hole transport material

Perovskite quality and bandgap:
- reproduce high-performance perovskite
- photo stable perovskite with a bandgap of 1.8 electron volts

Silicon cell:
- back contact scheme with lower SRV

C. D. Bailie, M. D. McGehee *MRS Bulletin*, 40 (2015) 681-5.

High bandgap perovskite model

Assumptions

- Current-matched to mc-Si cell with 1.74eV bandgap Maintain 0.37V Δ (1.19V Voc reported from 1.56 eV perovskite)[1]
- 1 µm material

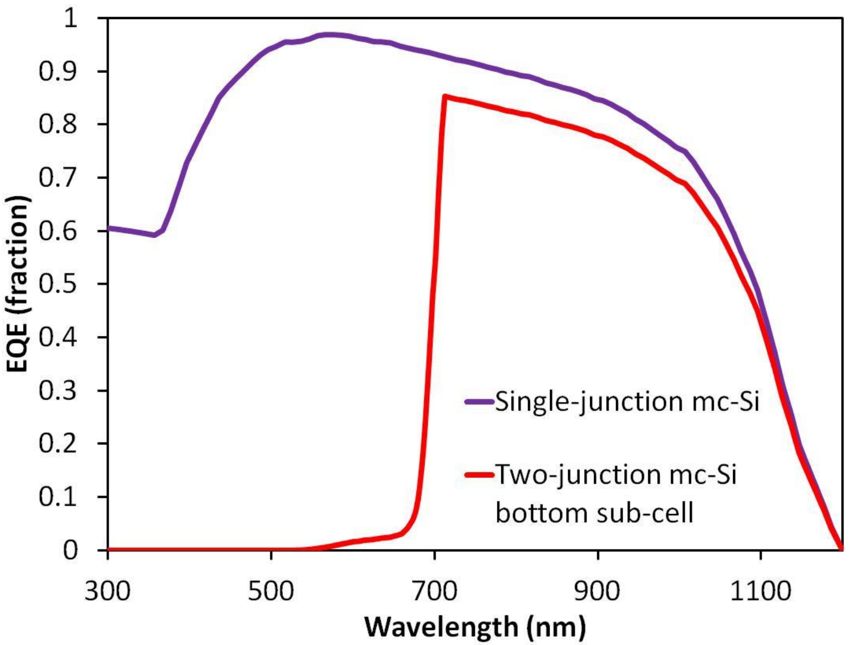
V_{OC}	1.37V
J_{SC}	18.3mA/cm2
FF	0.77
η	19.3%

1. J. P. Correa Baena, A. Hagfeldt, et al., *Energy Environ. Sci.* (2015).
2. P. Löper, C. Ballif, et al., *J. Phys. Chem. Lett.* **6**, 66–71 (2015).

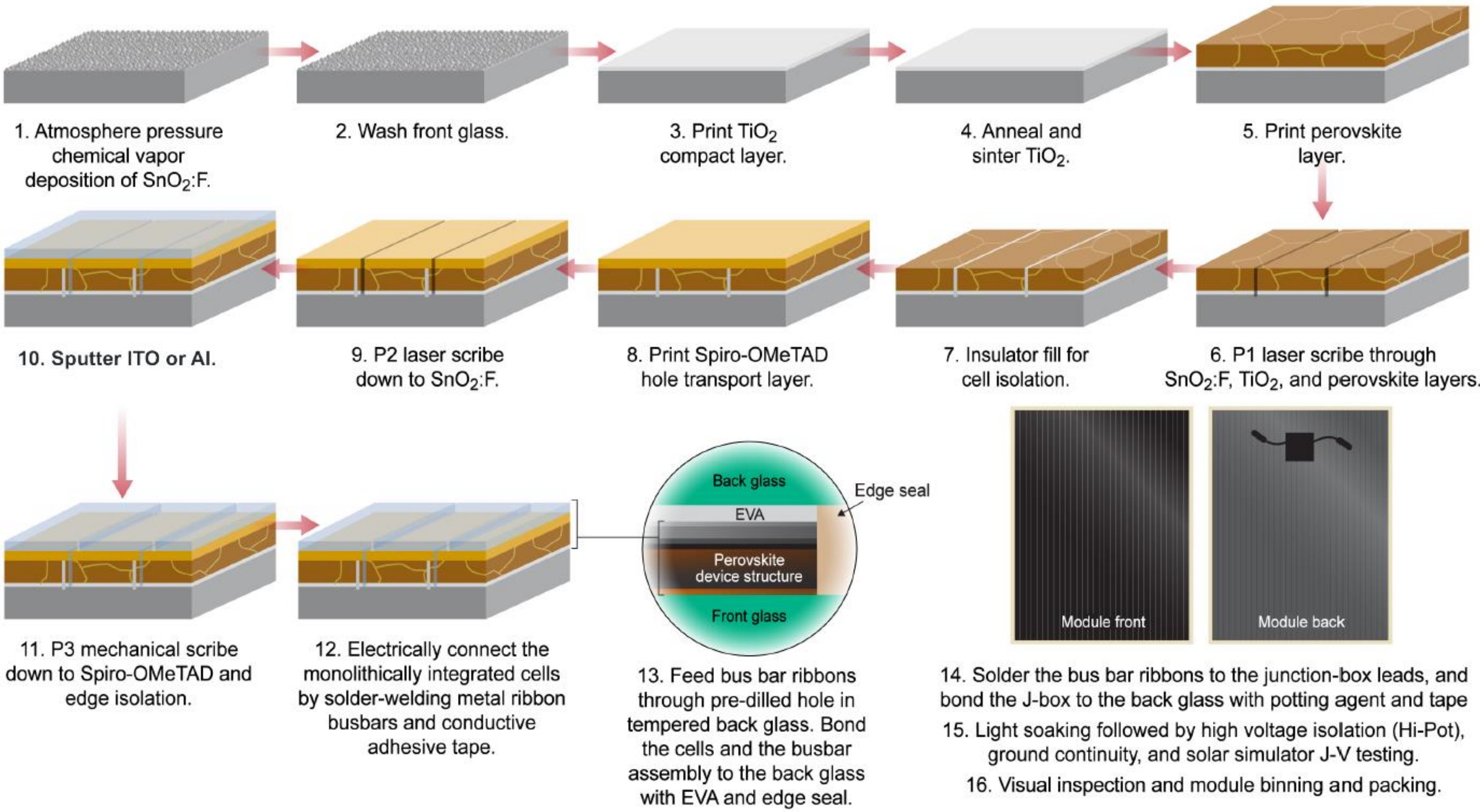
Tandem performance assumptions

- Standard mc-Si cell, 18% at AM1.5G
- Fitted to ideal diode equation with Rs and Rsh
- New J_{SC} using perovskite filter

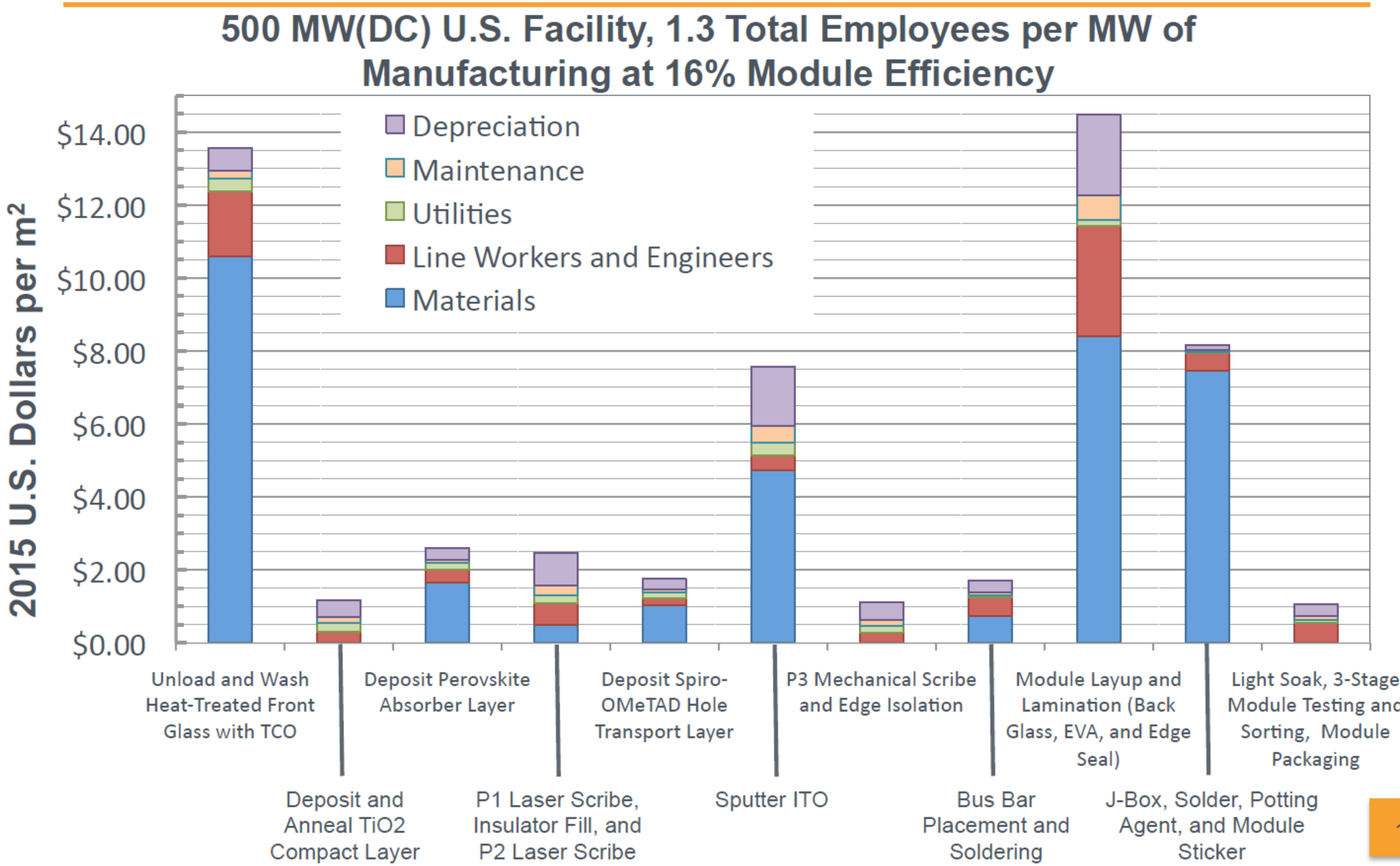
	AM1.5G	Filtered
V_{OC}	0.63V	0.60V
J_{SC}	38. mA/cm2	18.3 mA/cm^2
FF	0.75	0.77
η	18.0%	8.5%



Modelling the Process Flow for a 1J PSM similar to CdTe PV



Calculated Manufacturing Costs for 1J $MAPbI_3$ Module



Ongoing DRAFT NREL Analysis

Cost to upgrade to a tandem

Today's Si	+ Perovskite upgrade	Perovskite/Si Tandem
$0.51/W$_{DC}$		$0.34/W$_{DC}$
16% efficient		27.8% efficient
$82/m^2	+$13/m^2	$95/m^2