Organic photovoltaics:

Challenges and opportunities for theory, modeling, & simulation

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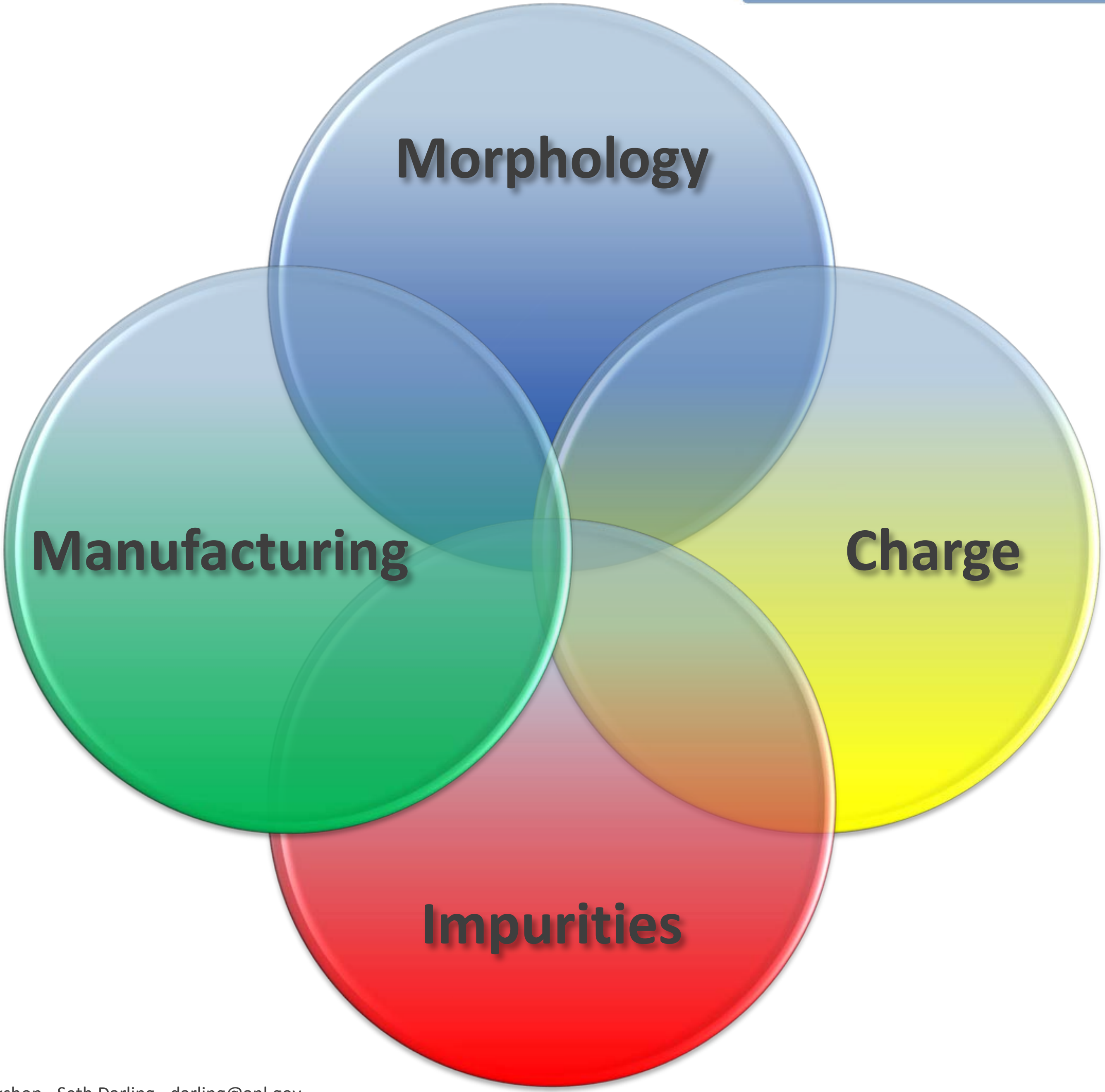
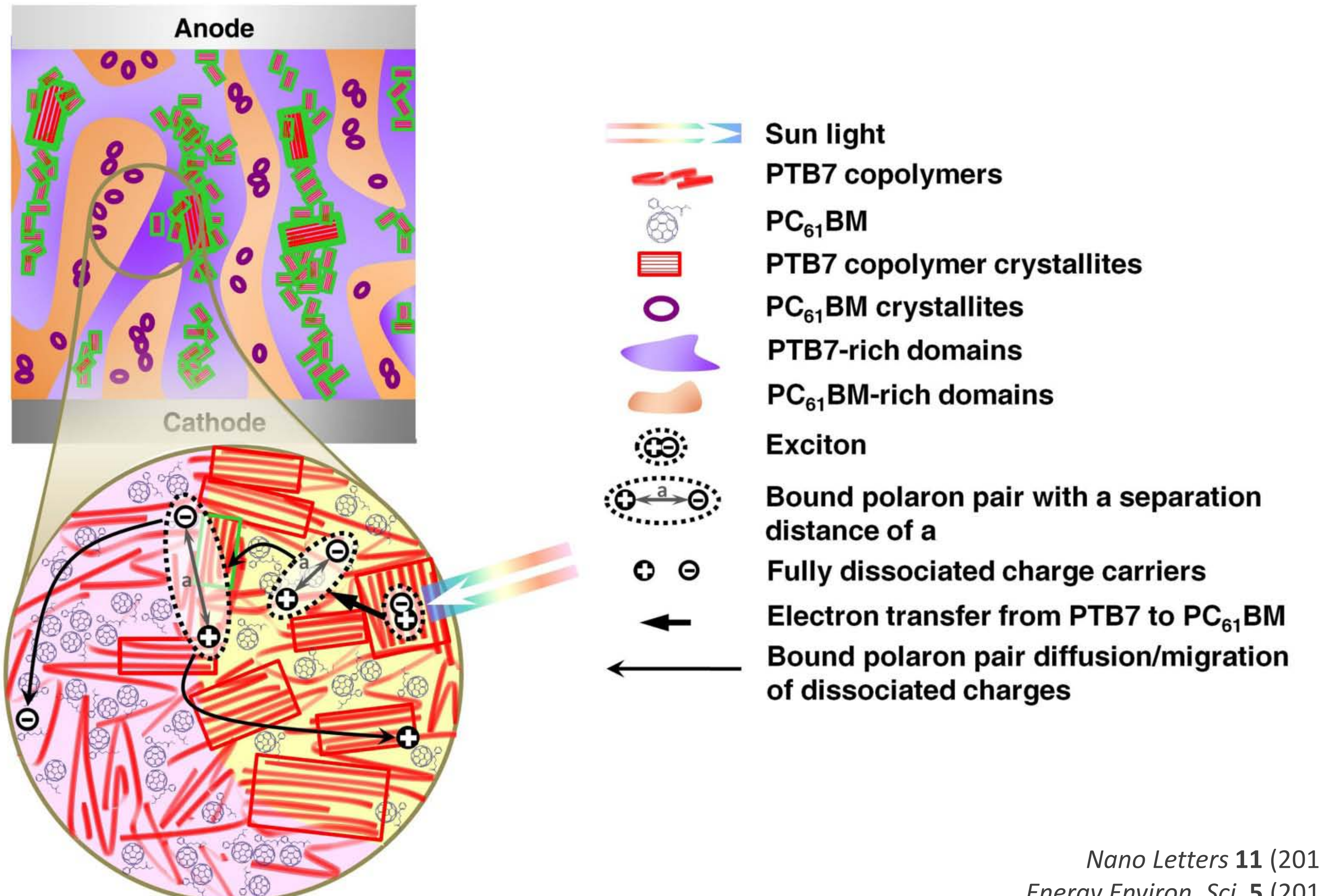

Morphology
Manufacturing
Charge
Impurities

Morphology

Hierarchical morphologies in the active layer



Nano Letters **11** (2011) 3707
Energy Environ. Sci. **5** (2012) 8045

Morphology

- How and when do each of these morphological features form?

in solution

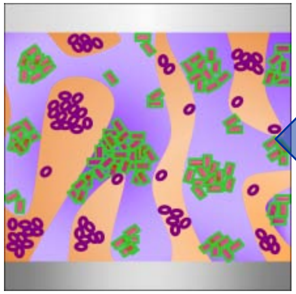
during deposition

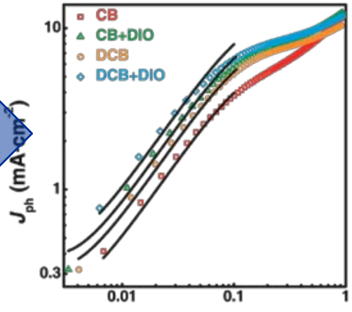
during annealing

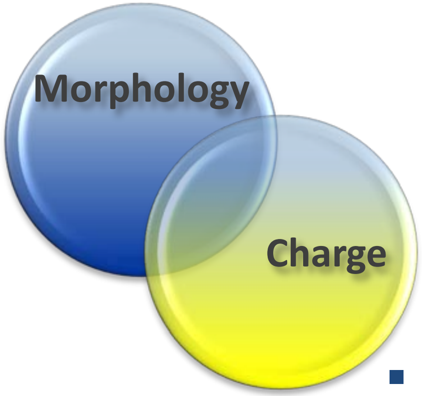
Morphology

Charge

- Correlation of morphology and performance: Charge separation





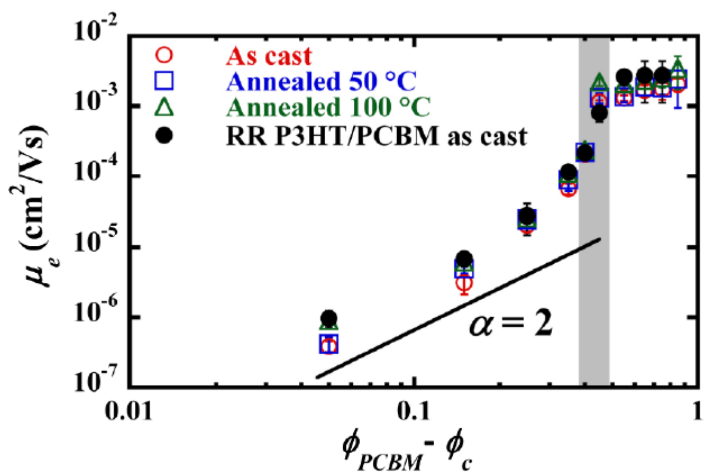


- Correlation of morphology and performance: Charge (polaron) transport
  - Carrier mobilities depend monotonically on miscibility for amorphous blends and can be described with percolation theory

$$(\phi - \phi_c)^{\alpha}$$

dimensionality factor

percolation volume fraction

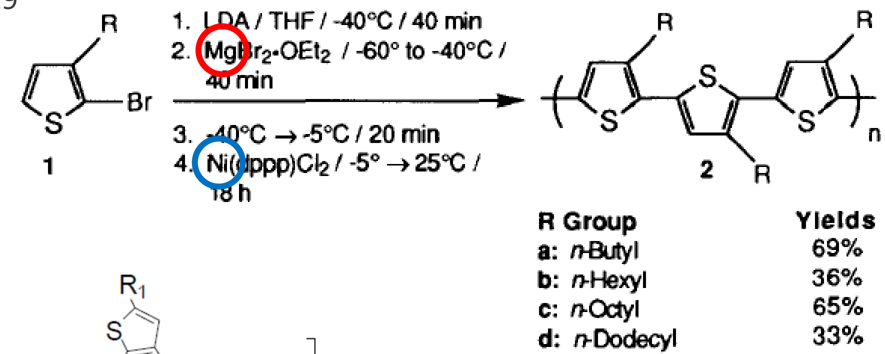


Phys Rev Lett **108** (2012) 026601

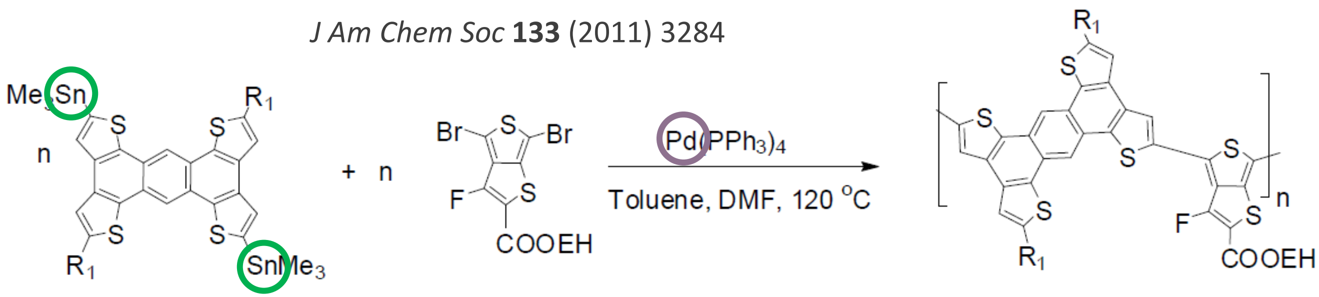
- Crystallinity adds complexity: good models for “real” OPV films remain elusive

Impurities

Synth Met **55** (1993) 119

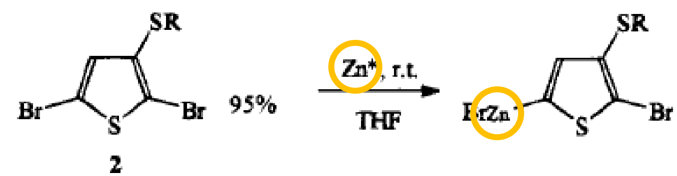


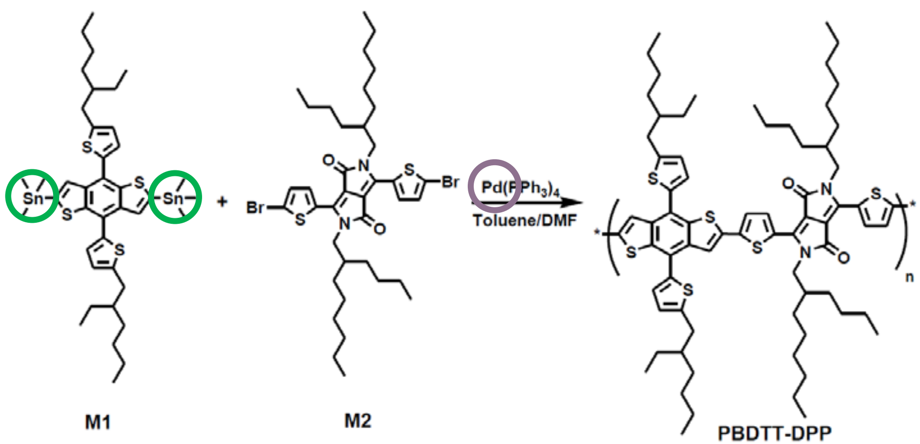
J Am Chem Soc **133** (2011) 3284



PTTATT-X

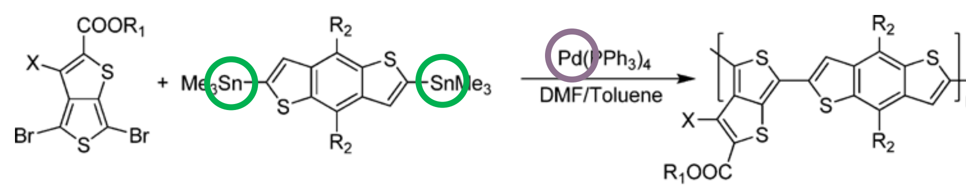
Macromolecules **28** (1995) 2101





Nature Photonics **6** (2012) 180

Acc Chem Res **43** (2010) 1227

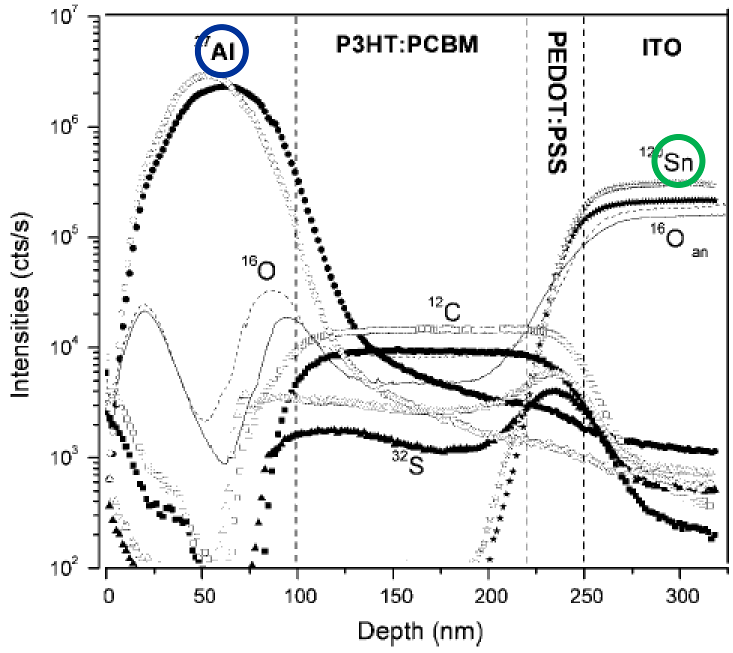


PTB1: X = H, R_1 = n-dodecyl, R_2 = n-octyloxy
PTB2: X = H, R_1 = 2-ethylhexyl, R_2 = n-octyloxy
PTB3: X = H, R_1 = 2-ethylhexyl, R_2 = n-octyl

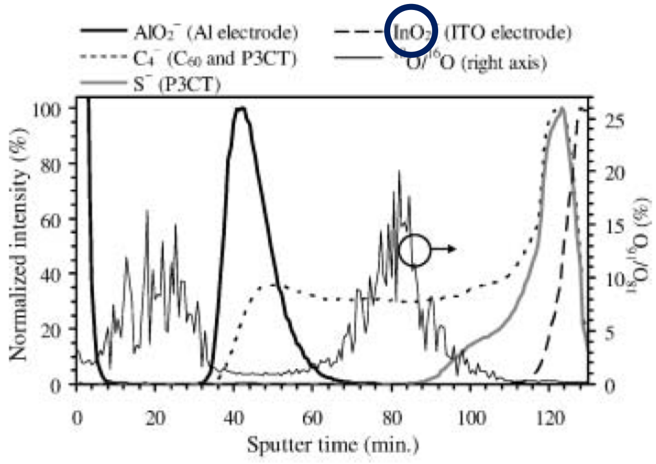
PTB4: X = F, R_1 = n-octyl, R_2 = 2-ethylhexyloxy
PTB5: X = H, R_1 = n-octyl, R_2 = 2-ethylhexyloxy
PTB6: X = H, R_1 = 2-butyloctyl, R_2 = n-octyloxy

Impurities

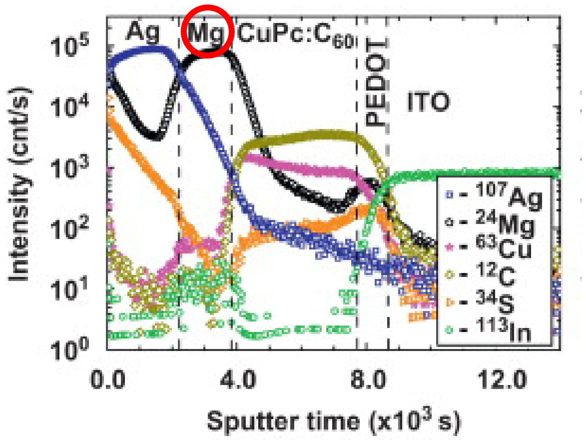
- Diffusion of electrode materials into active layer



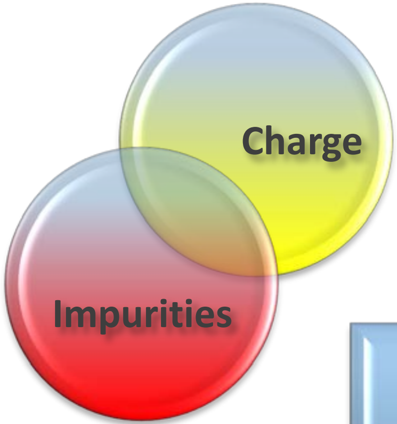
Surf Interface Anal **42** (2010) 1010



Prog Photovolt: Res Appl **15** (2007) 697

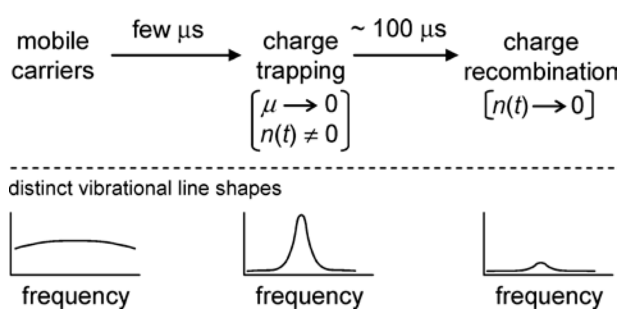


Sol Energy Mater Sol Cells **95** (2011) 1489

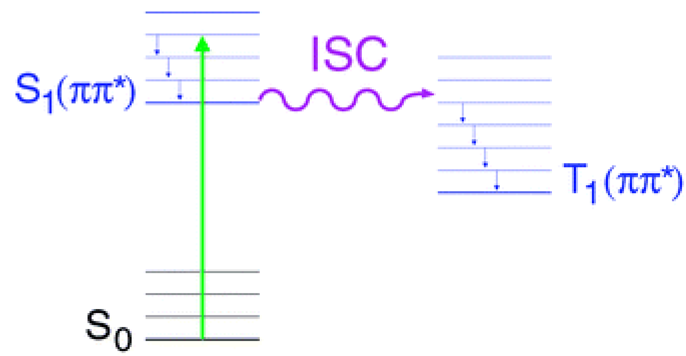


- What, if any, role do these impurities play?

Bad?	Good?
• Charge trapping	• Triplet conversion



J Phys Chem C **114** (2010) 5344



- Work function gradient?

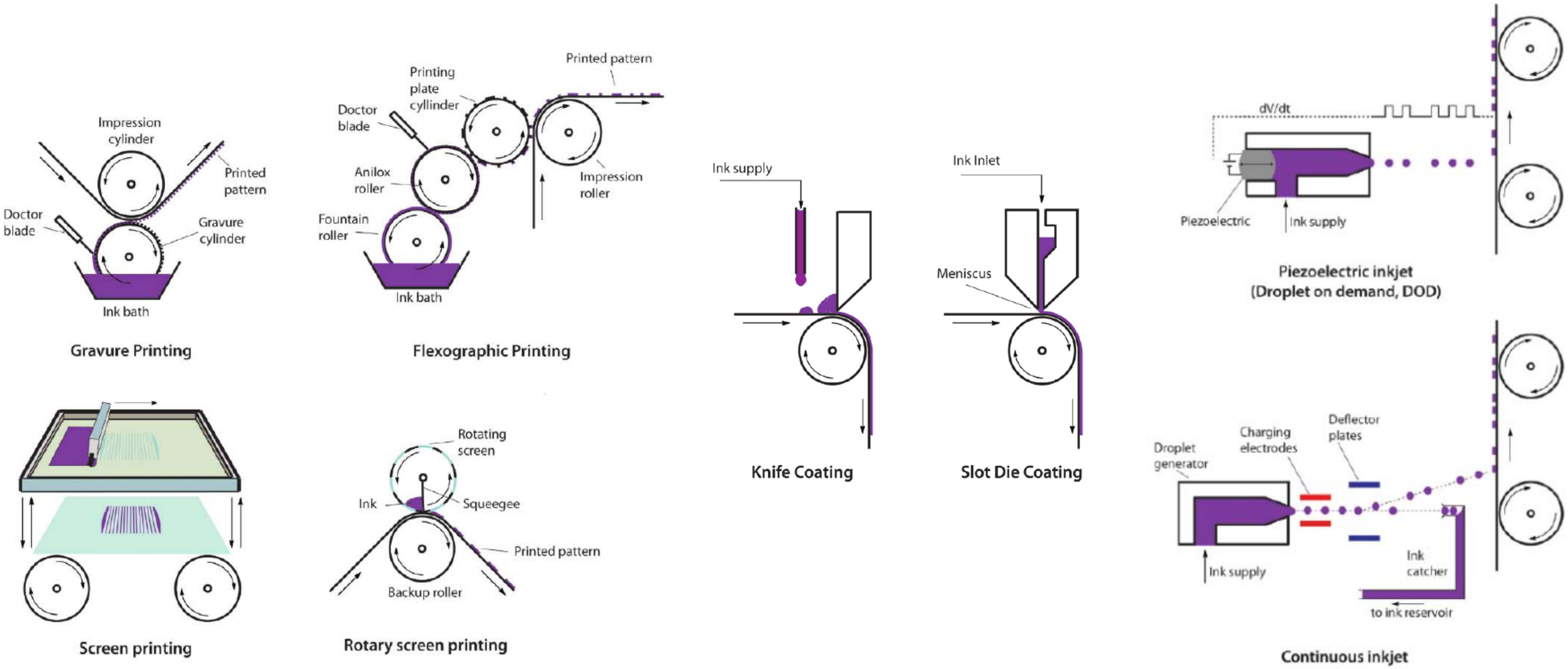
Manufacturing

- Performance gap for OPVs is far larger than for traditional PVs

PV technology	Lab record cell PCE*	Commercial module PCE	% Decrease
c-Si	25.0	20.1 (SunPower)	19.6
p-Si	20.4	14.6 (Schott)	28.4
a-Si	10.1	5.1 (Uni-Solar)	49.5
CIGS	19.6	12.5 (Q-Cells)	36.2
CdTe	16.7	12.5 (First Solar)	25.1
DSSC	11.0	1.74 (G24 Innovations)	**84.2**
OPV	10.0	1.65 (Konarka)	**83.5**

* *Prog. Photovolt.: Res. Appl.* **20** (2011) 12

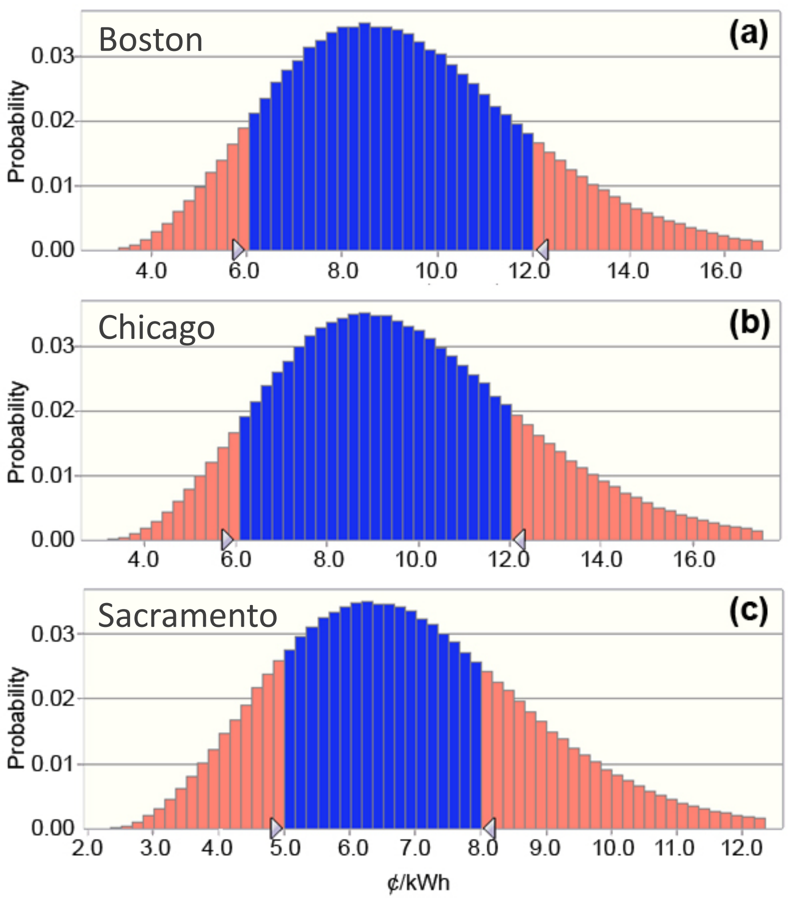
- Deposition techniques are connected with morphology
  - Model kinetics of evolution during solvent evaporation
  - Model role of solvents & additives (viscosity tuning)

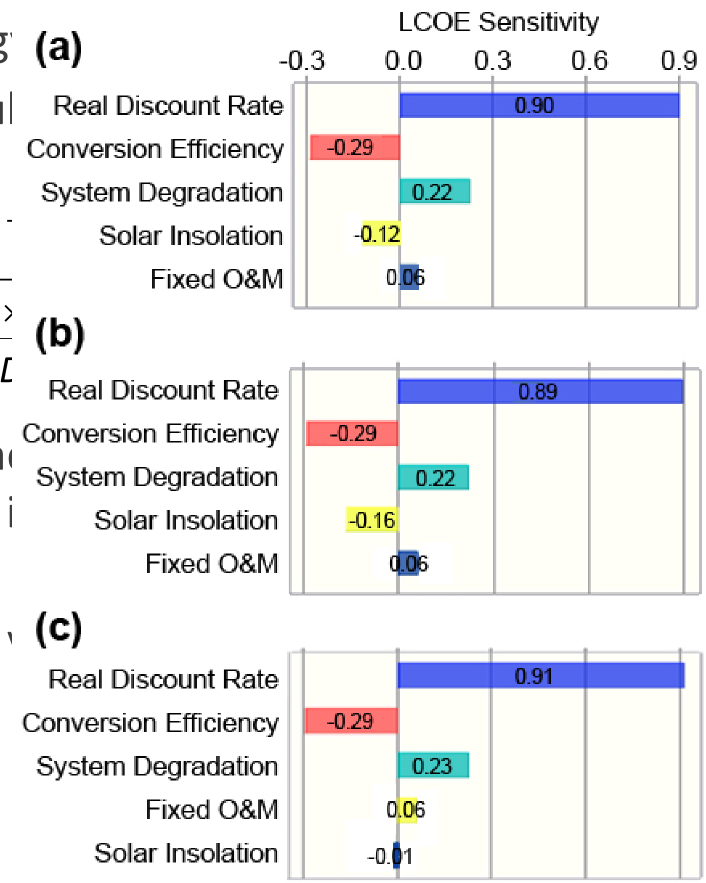


Mater. Today **15** (2012) 36
MRS Bulletin **30** (2005) 50

Manufacturing

Levelized cost of energy (LCOE)



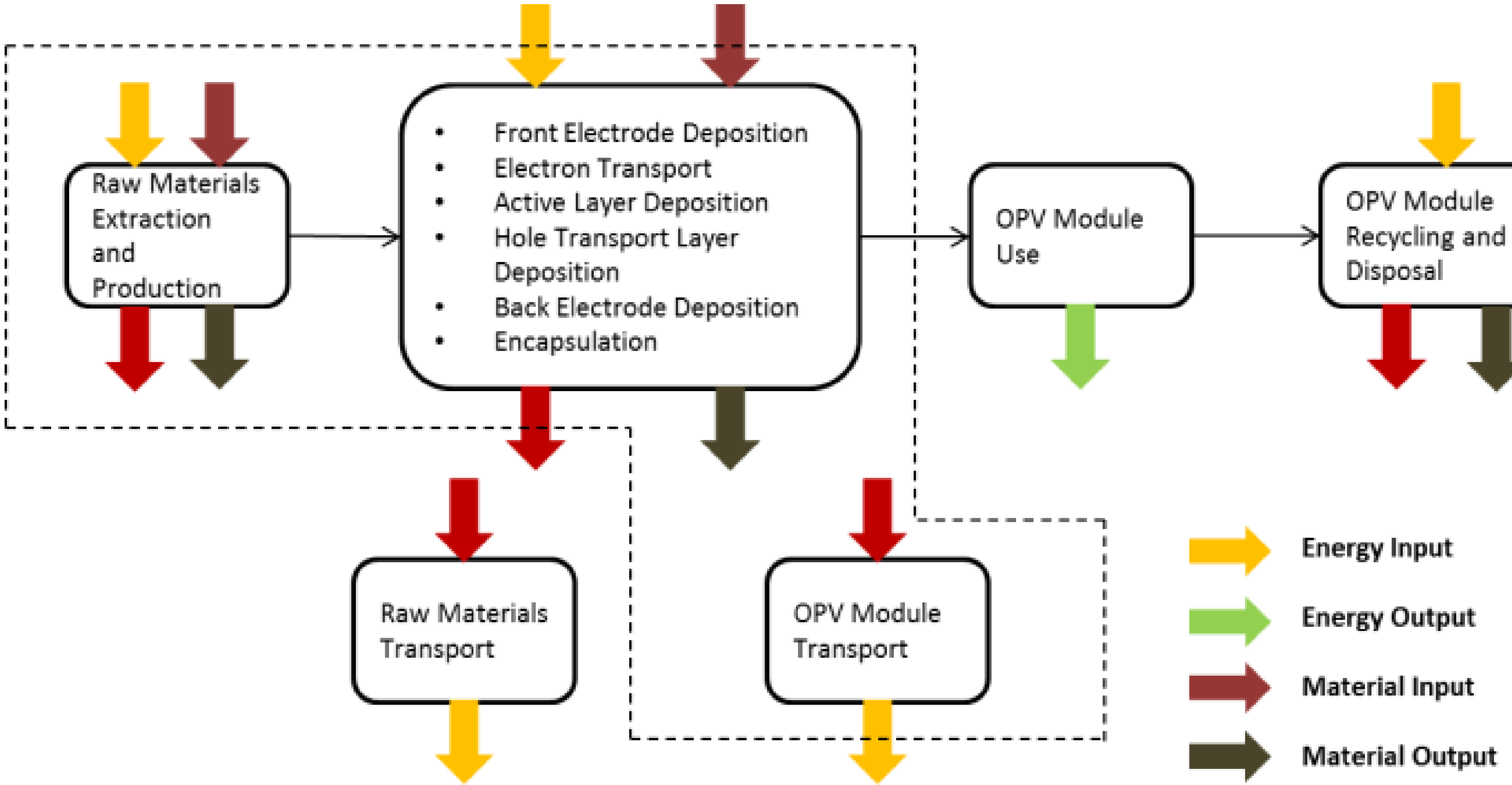


- Growing need for analogous analysis for OPVs

Energy Environ Sci **4** (2011) 3133

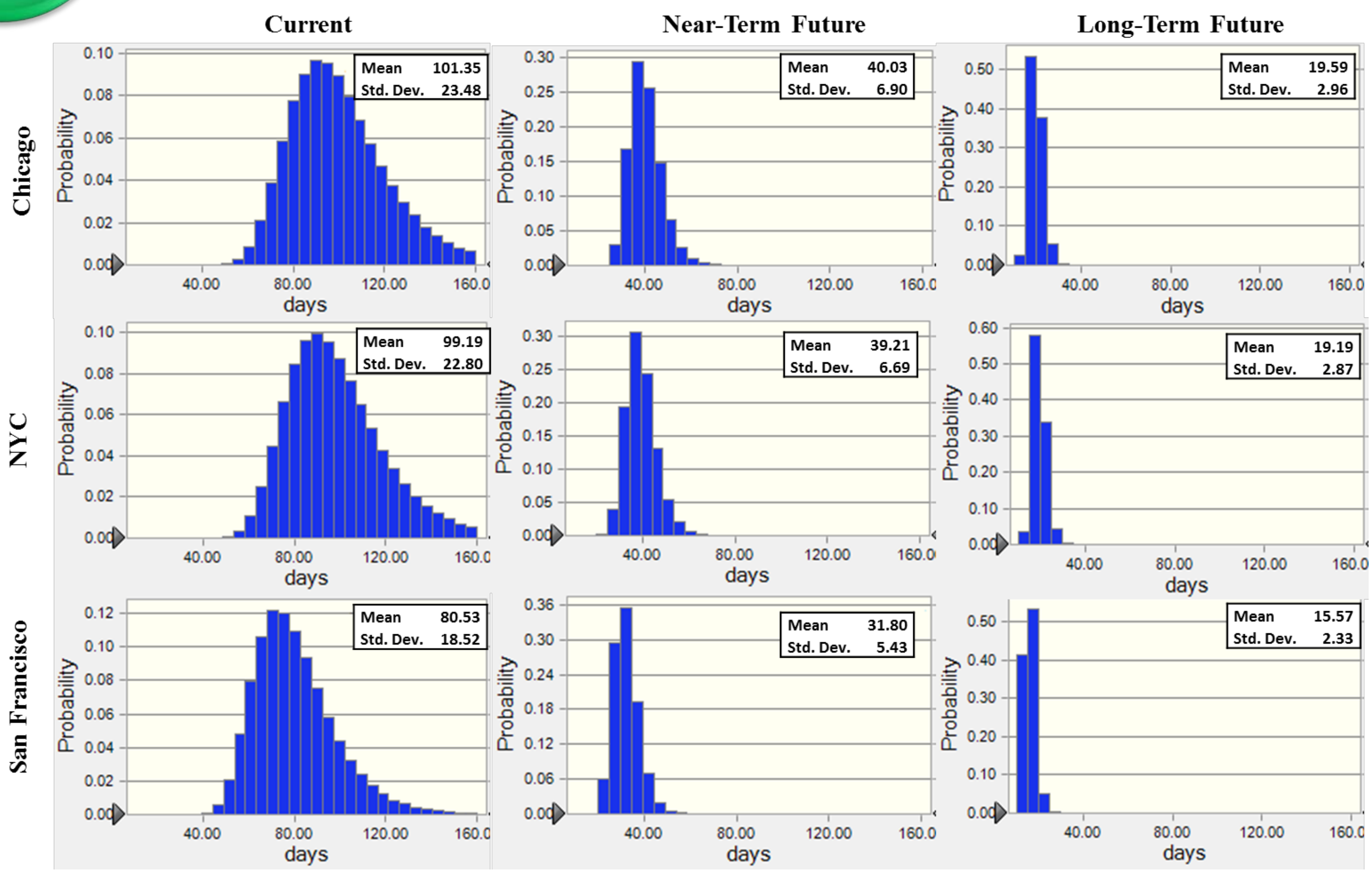
Manufacturing

Life cycle analysis (LCA)



Manufacturing

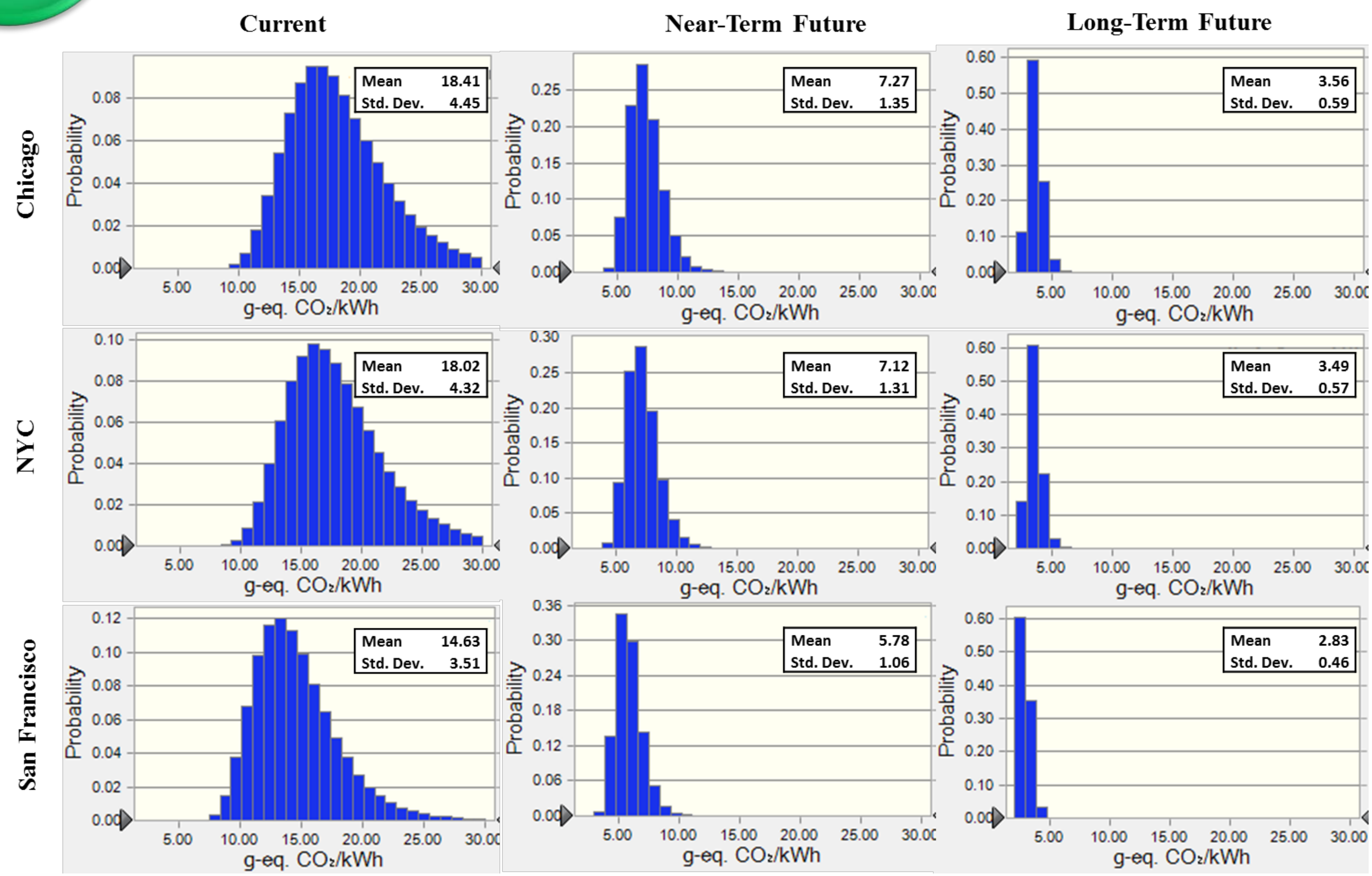
Energy payback time (EPBT)



Energy Environ Sci Submitted

Manufacturing

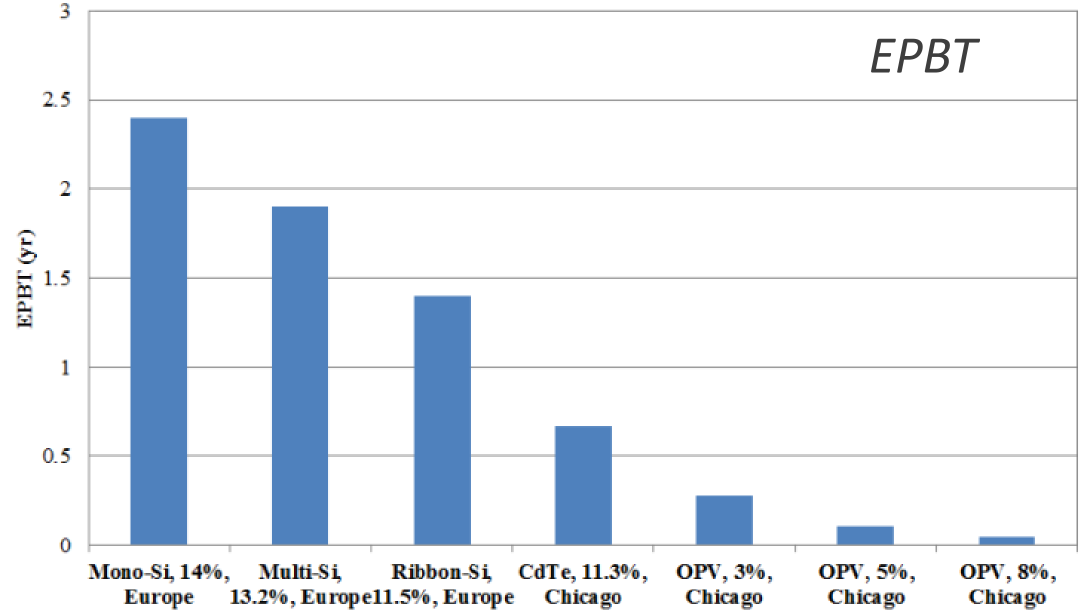
Carbon emissions

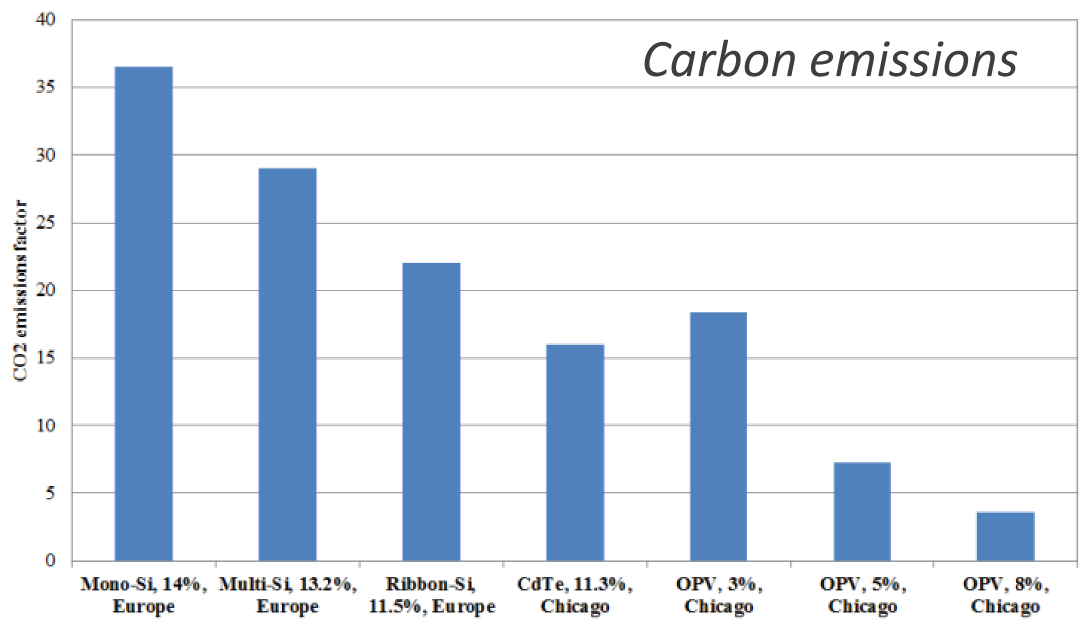


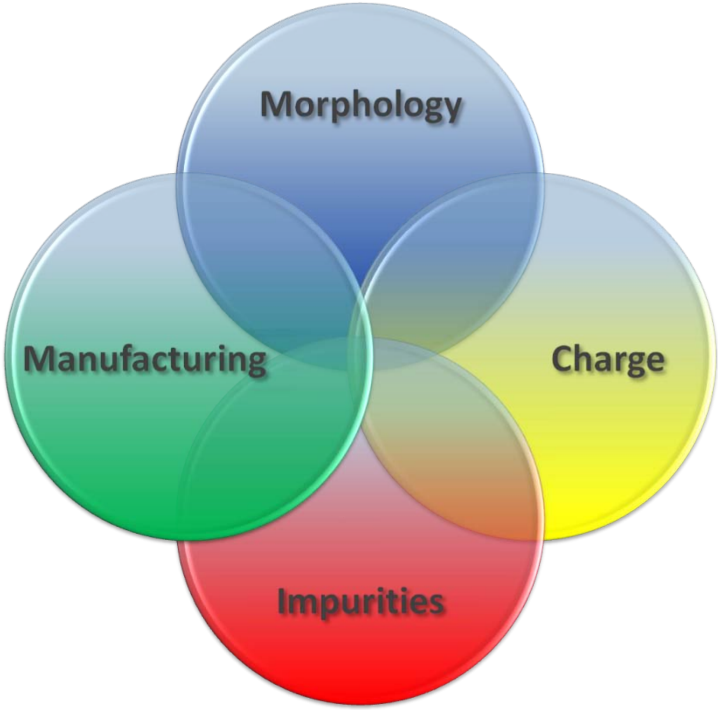
Energy Environ Sci Submitted

Manufacturing

- Making the case for OPV as a commercial technology will require careful LCA analyses
- Initial studies are encouraging







- Morphology formation mechanisms
- Morphology-function relationships
- Charge separation process
- Role of impurities/dopants
- Life cycle analysis