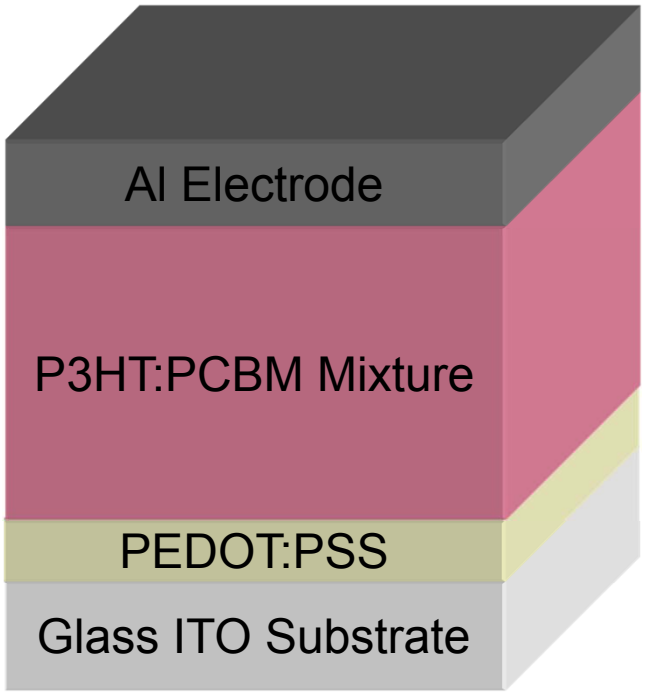
Understanding Morphology: How measurement affects perception

Scott A. Mauger, John Roehling, Lilian Chang, Stephan Friedrich, Christopher W. Rochester, David M. Huang, Peng Wang, Jaroslaw Majewski, and Adam J. Moulé

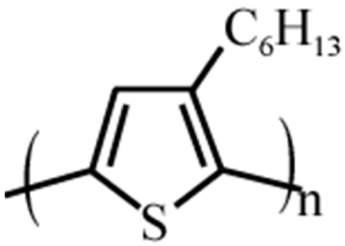
UC Solar 2013

Davis, CA

How does it work?

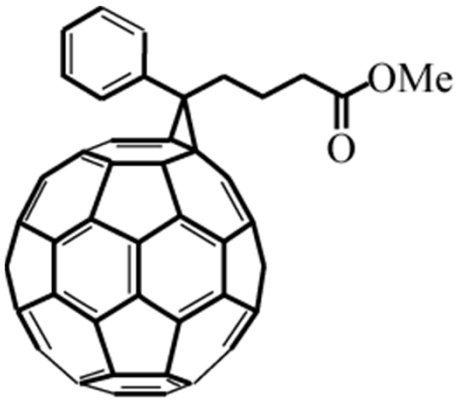


Electron Donor



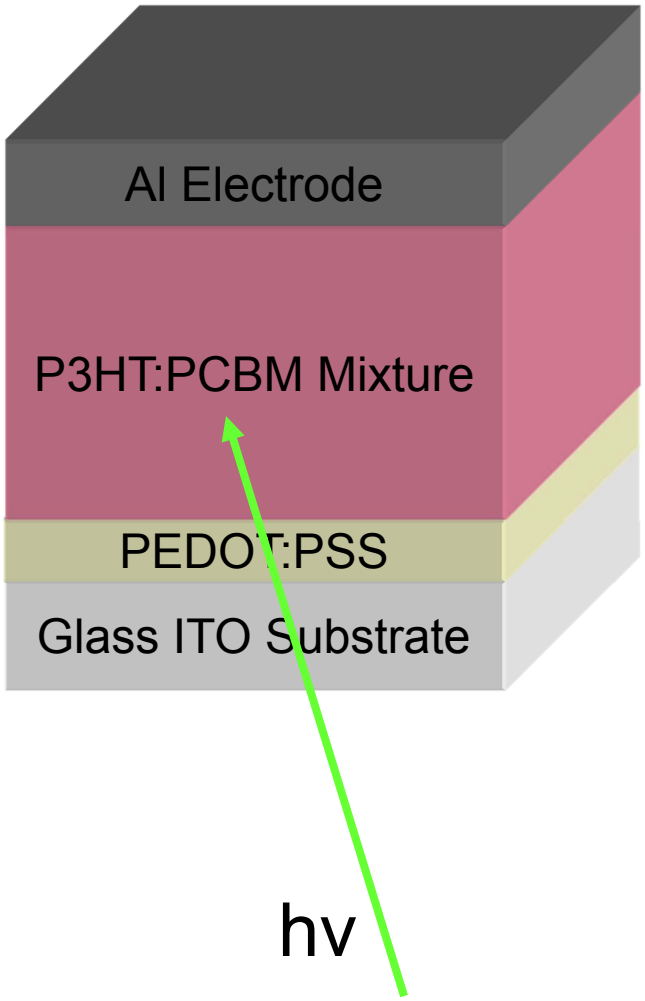
P3HT

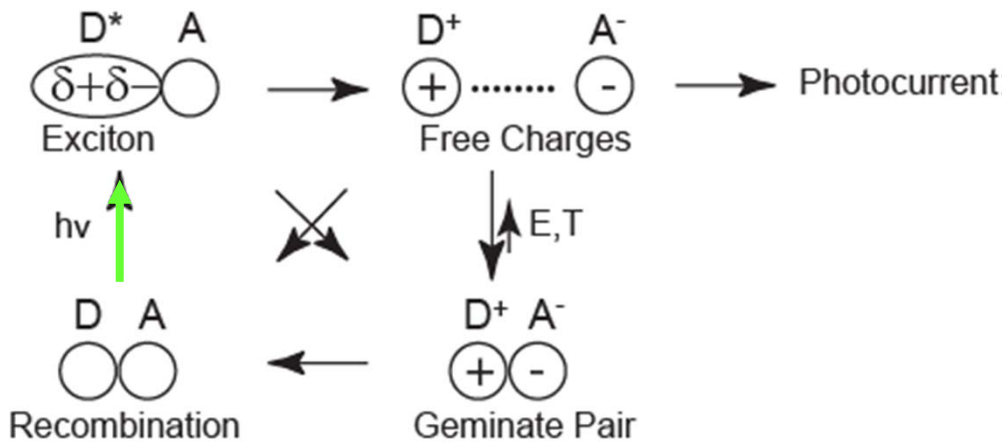
Electron Acceptor

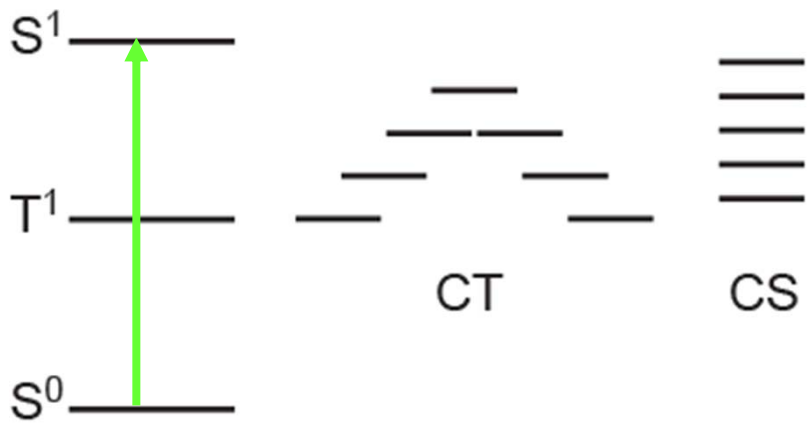


PCBM

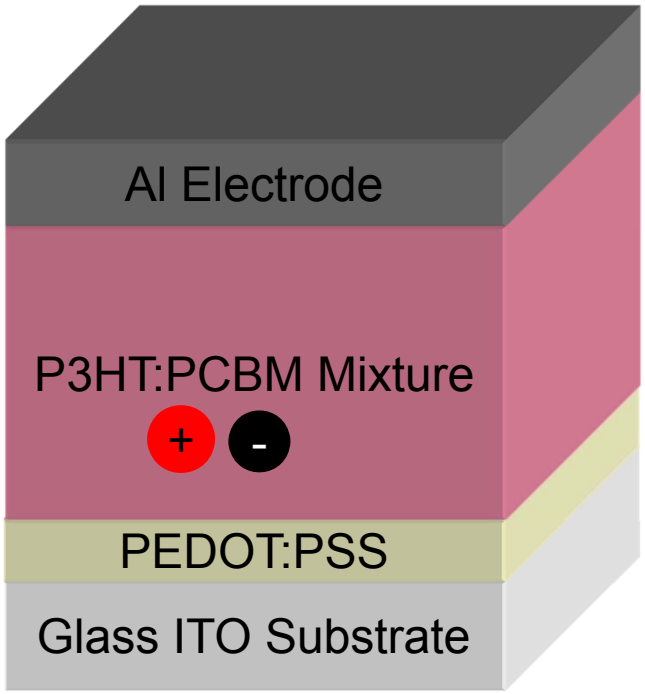
How does it work? - Excitation

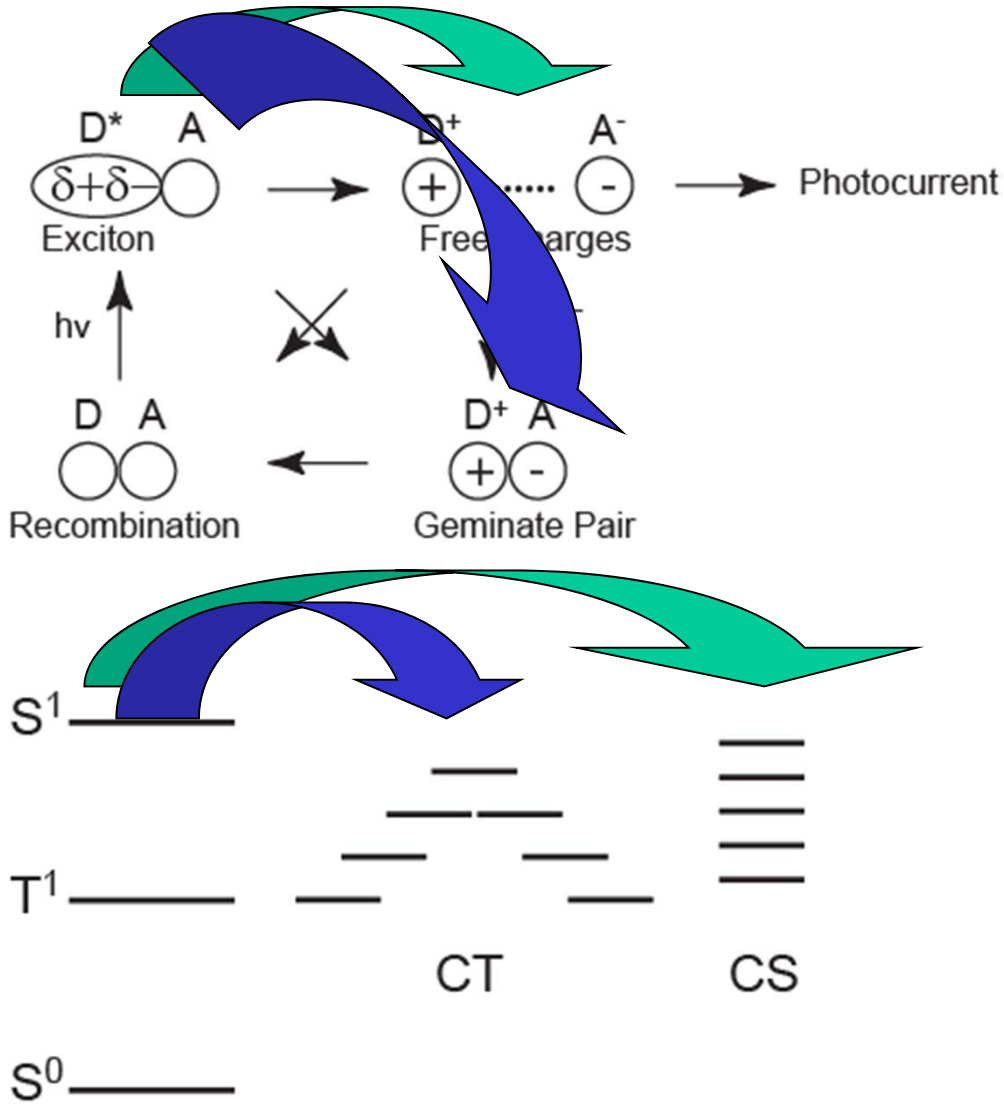




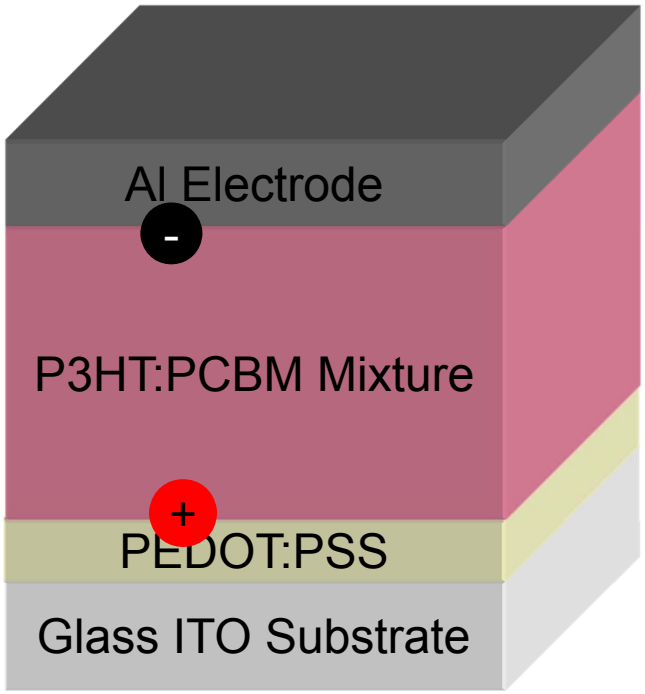


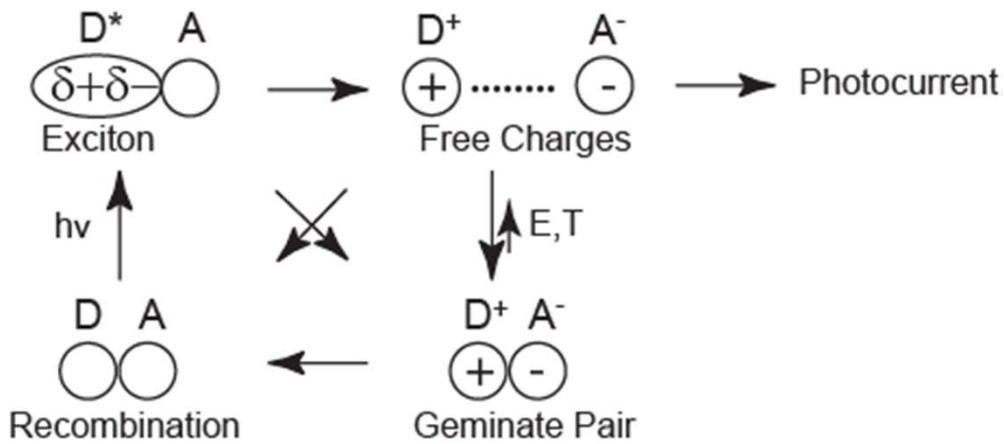
How does it work? – Charge transfer

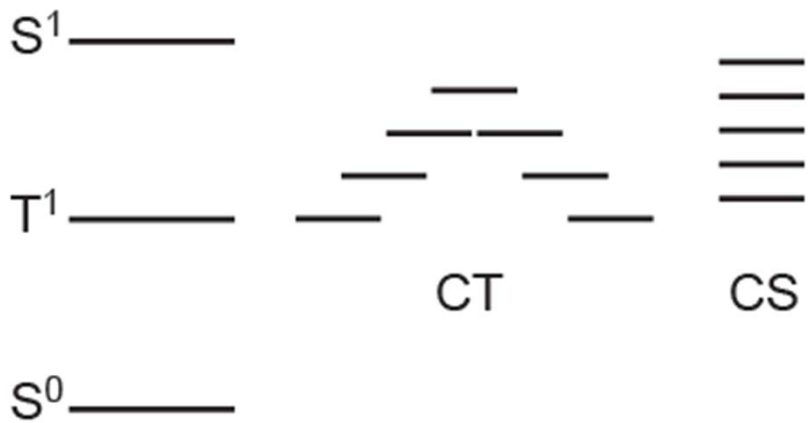




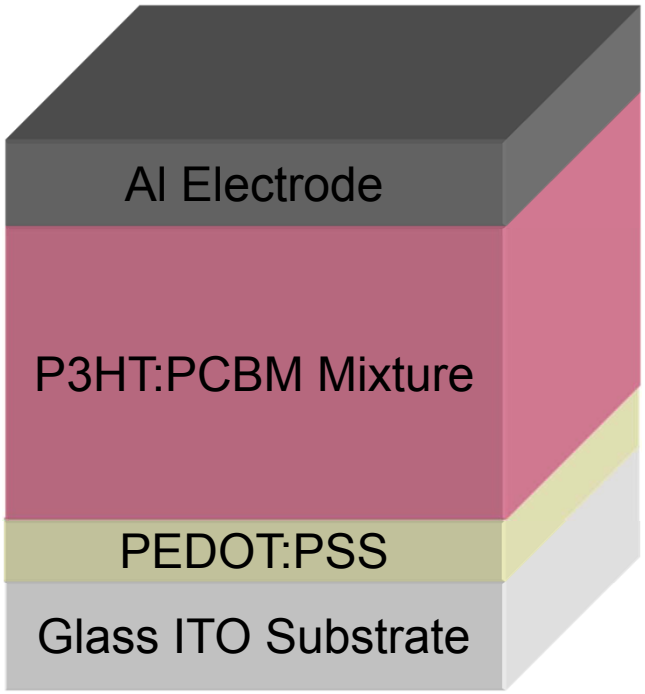
How does it work? - photocurrent

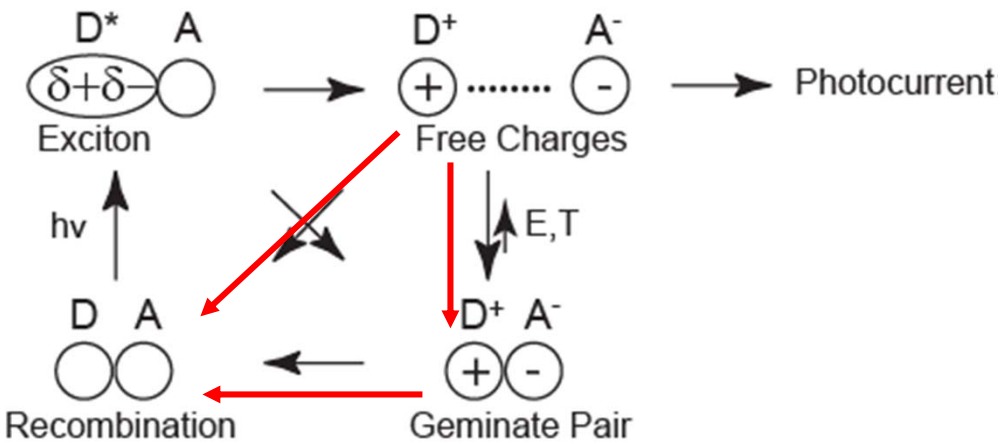


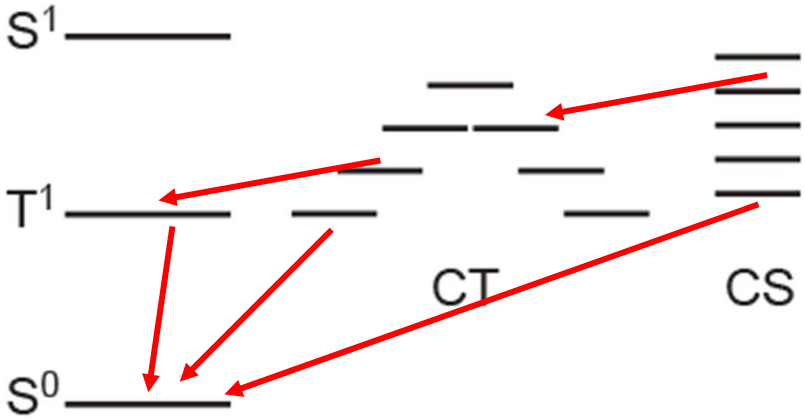




How does it work? - recombination







Chemical Physics Letters 2011, 513, 77

Journal of Physical Chemistry Letters 2011, 2, 2764.

So, can this picture explain OPV device function

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So, can this picture explain OPV device function

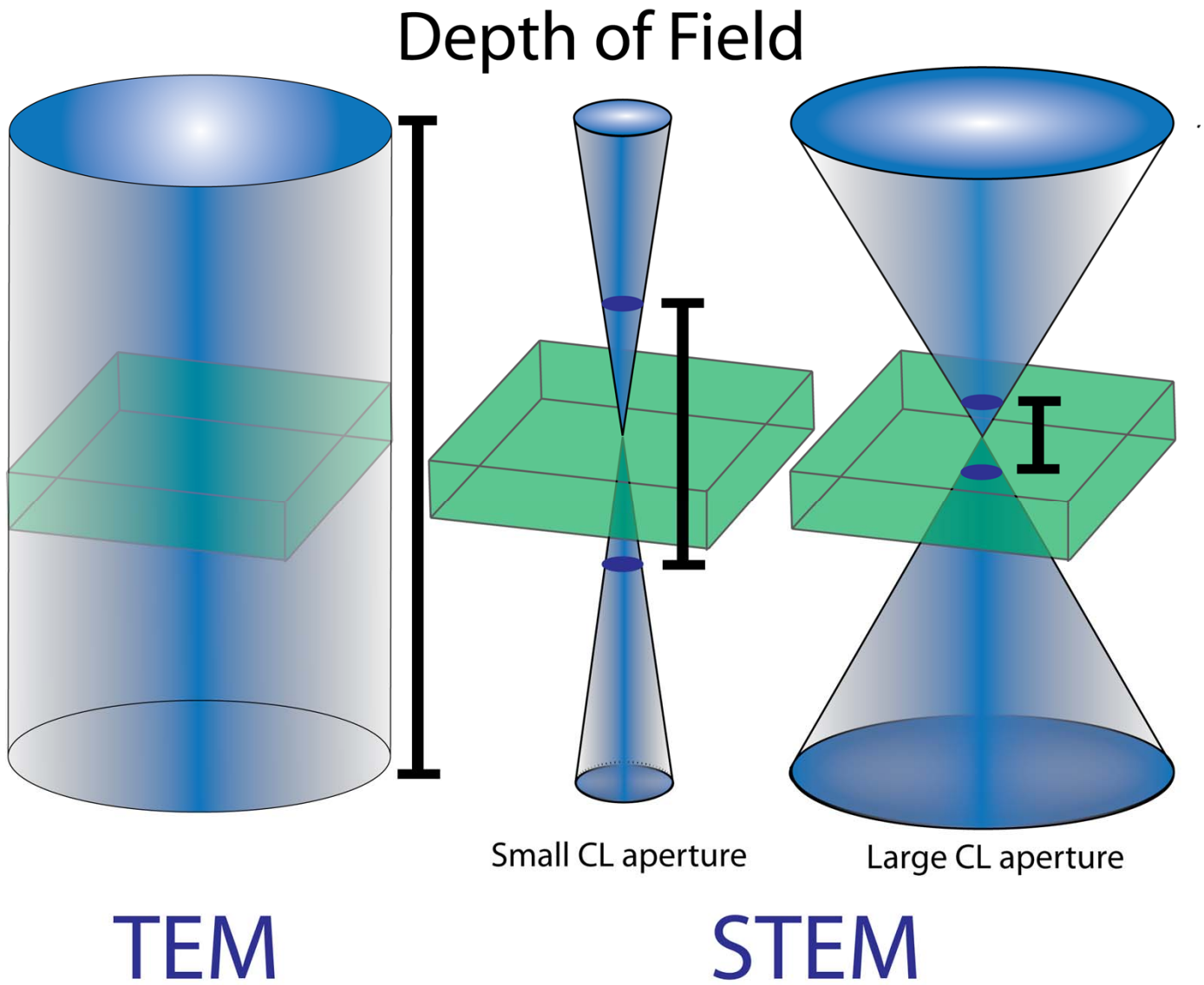
Almost

What about Morphology?

Morphology Challenges

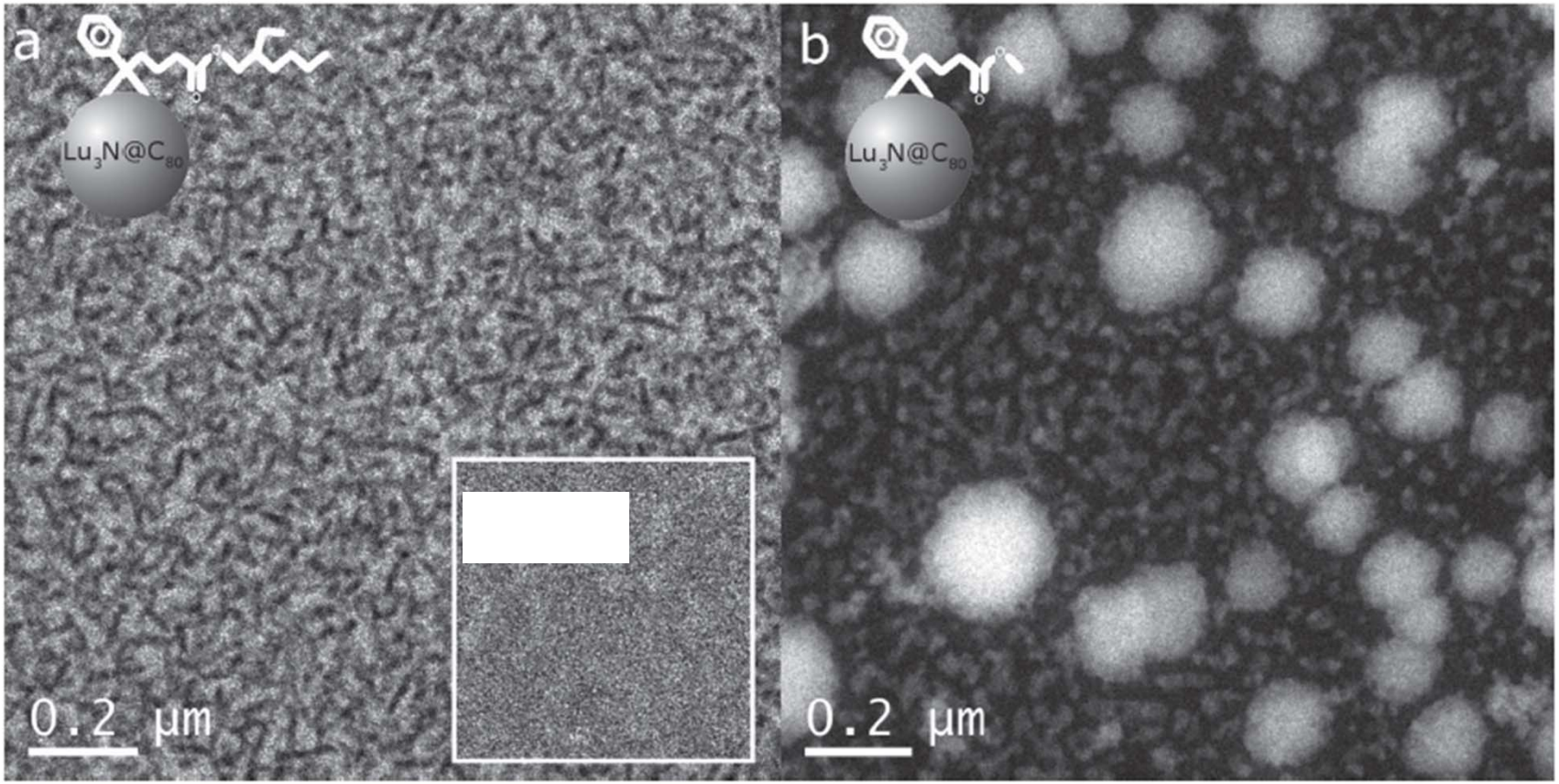
1) Domain sizes are <50 nm and so cannot be seen with light
2) There is little scatter contrast between carbon containing materials, SAXS and GWAXS have low signal
3) The materials are semi-crystalline so much of sample is invisible to bragg scattering
4) Surface properties cannot be assumed to be uniform throughout the film so surface techniques give misleading results
5) The sample is highly sensitive to processing conditions, So it is difficult to get a generalizable result.
6) Most spectroscopy is performed on samples that were not produced under the same conditions as a device – no metal and no electrodes

TEM vs. STEM



Creating Contrast

Lu_3N-$PC_{80}BEH$ **Lu_3N-$PC_{80}BM$**



J. D. Roehling, K. J. Batenburg, F. B. Swain, A. J. Moule, I. Arslan, Accepted in Advanced Functional Materials 2013.

3D-Morphology of P3HT/Lu_3N-$PC_{80}BEH$

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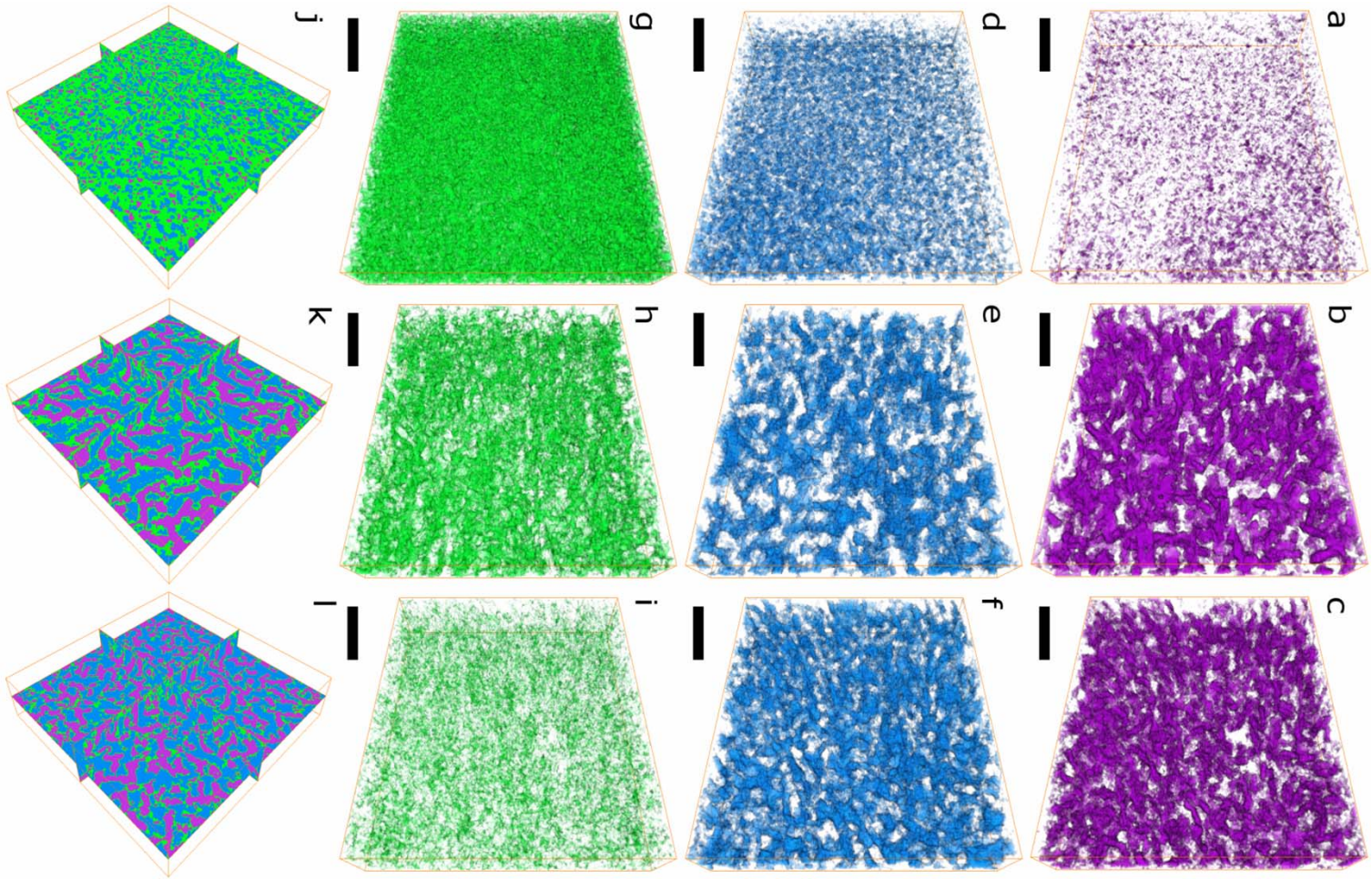
Full **Mixed** **Fullerene** **P3HT**



As-cast

Solvent Anneal

Thermal Anneal

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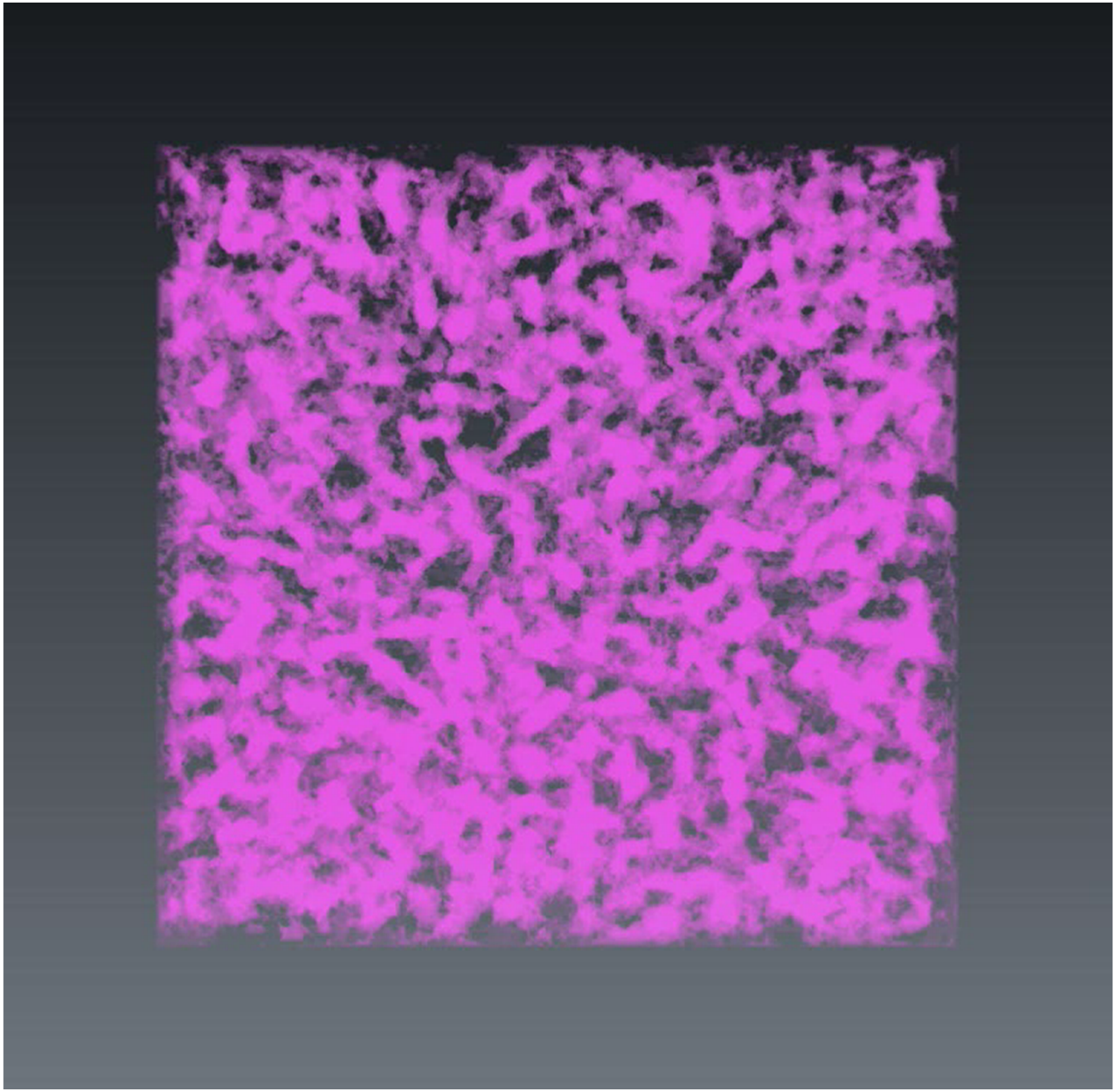
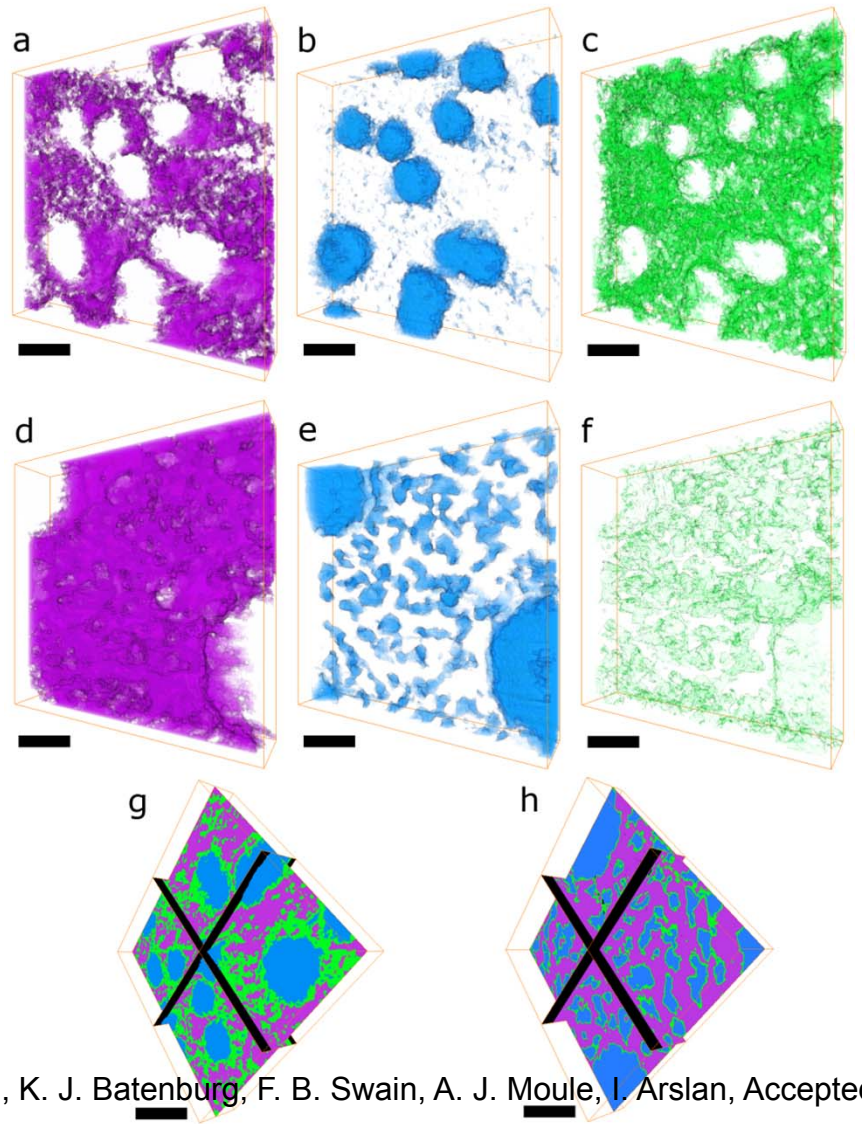
3D P3HT Domains



Morphology of P3HT/Lu_3N-$PC_{80}BM$

P3HT **Fullerene** **Mixed**



As-cast

Thermal Anneal

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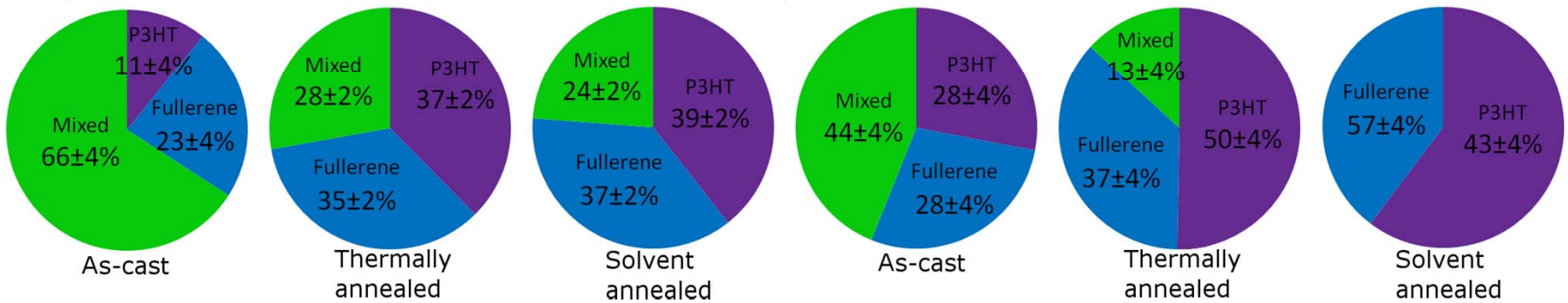
Quantifying Morphology

	Lu-PCBEH			Lu-PCBM		
% Vol Fullerene Mixed Phase	30±7	43±4	31±4	31±7	55±7	~0
% Vol Fullerene Fullerene Rich Phase	78±7	86±4	94±4	95±7	96±7	~100



Why are they so different?

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Crystallinity is bad!

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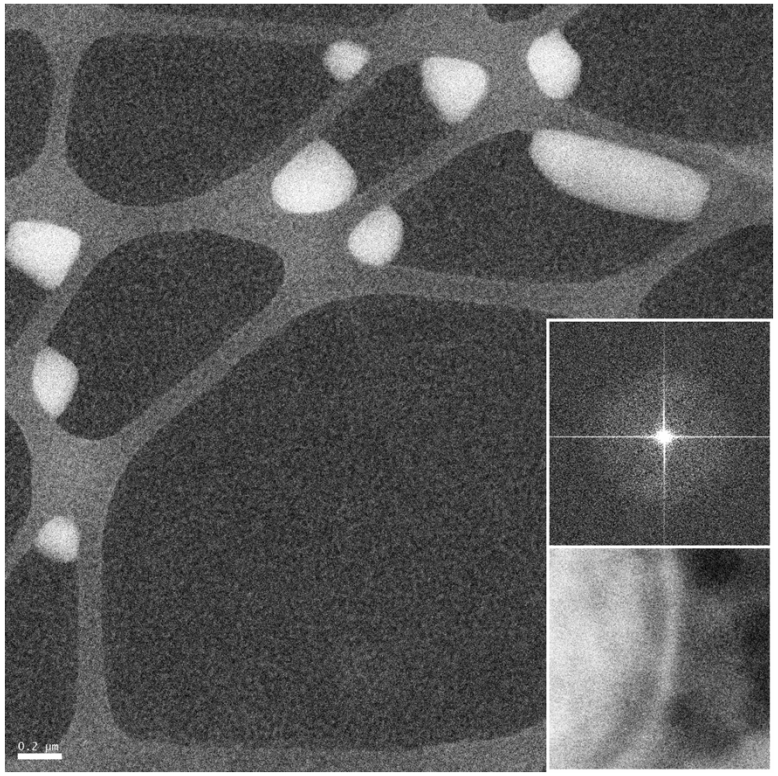
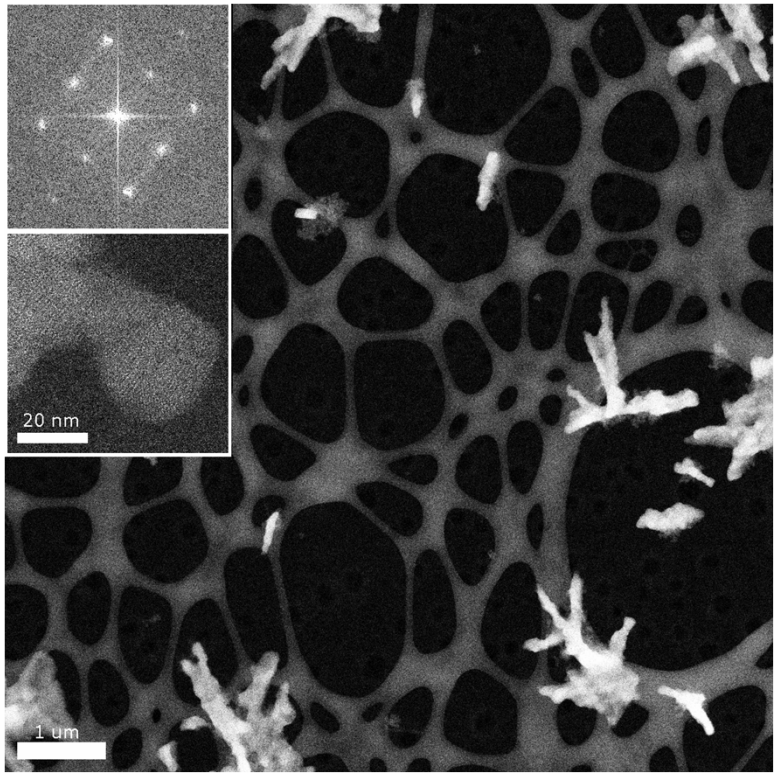
SA – P3HT/Lu_3-PC_{80}BEH



SA – P3HT/Lu_3-PC_{80}BM



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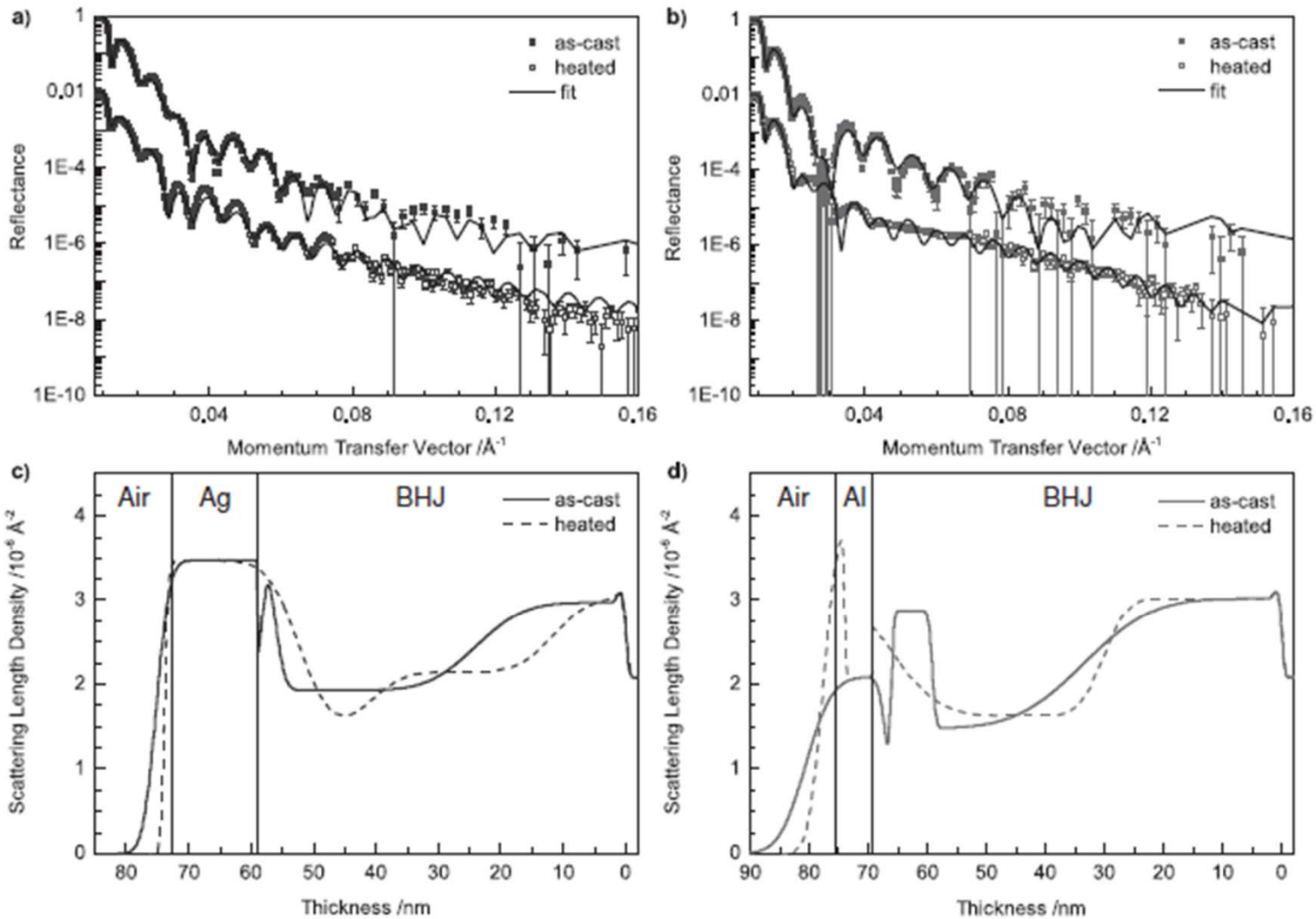
Real devices

Neutron Reflectometry



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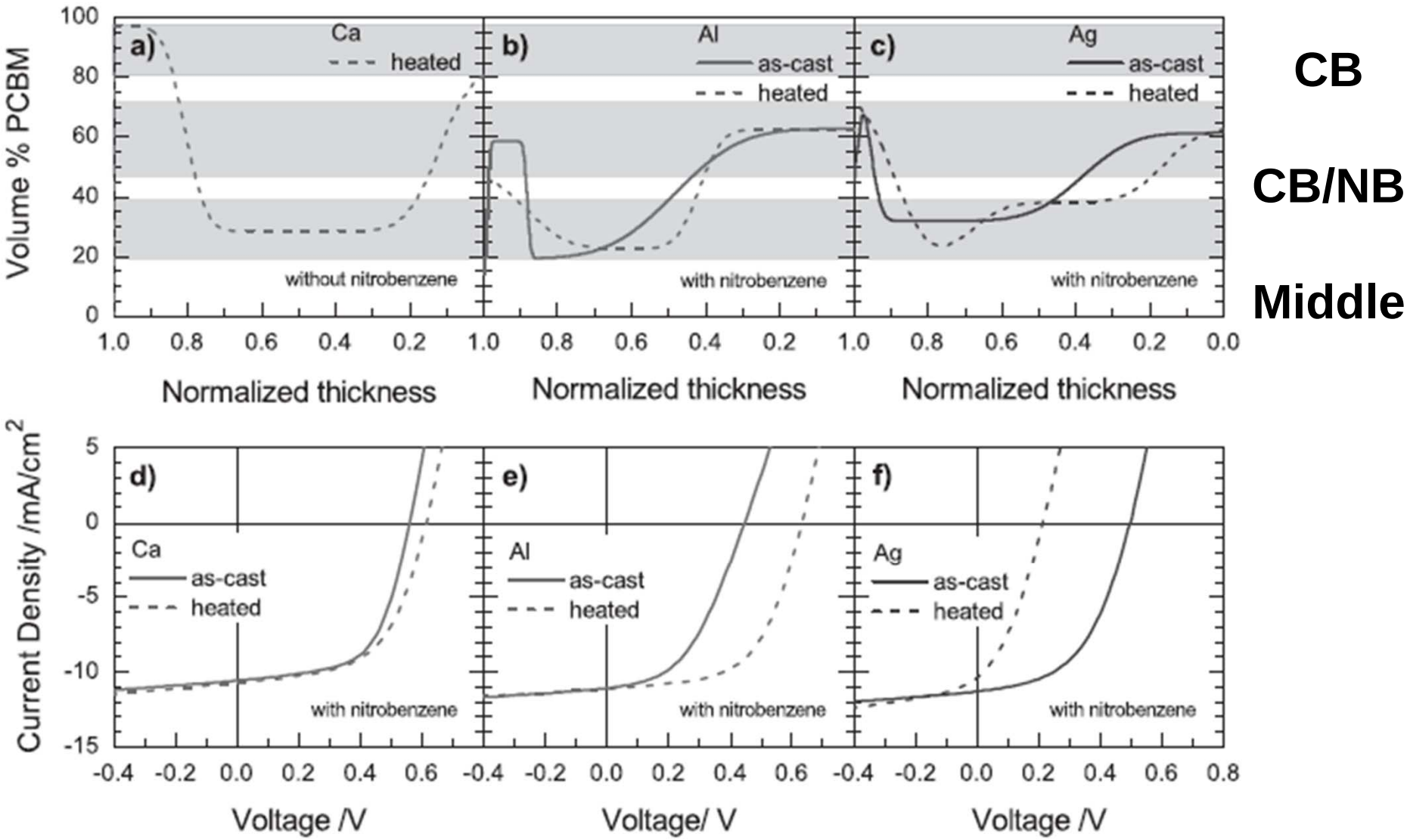
Vertical Segregation in a device



CB

CB/NB

Middle

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Why does vertical segregation occur?

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P3HT and PCBM rearrange upon annealing because of

1) Surface energy effects
2) Charging from interfaces (metals or PEDOT:PSS)
3) Choice of solvents and solvent additives

Why should you care?

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<u>These Images</u>

1) Have the highest resolution of any image ever taken of a BHJ layer 1.4x1.4x1.4 nm = $5x10^7$ voxels

2) Prove that a three phase diagram is necessary to describe the morphology

3) Quantify concentration at the nanoscale for the first time

4) With NR quantify the vertical and lateral phase segregation for the first time

5) Give us the ability to relate real nanostructure to optical and electrical properties.

Credits

UC Davis

Scott Mauger
Chris Rochester
John Roehling

LANL
Jarek Majewski
Peng Wang

Collaborators:
Prof. Delmar Larsen
Erik Busby

UC lab Fee – Roehling

NSF G K-12 RESOURCE Grant

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Thank you for your attention