Area Detector Diffraction: Small Molecule OSCs

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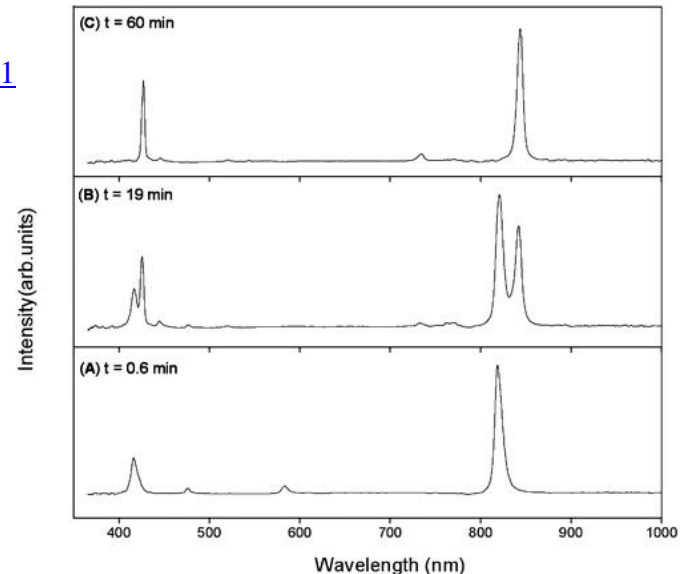
Stanford University

Kinetic Crystallization

- Crystallization away from chemical potential equilibrium
- Different properties than equilibrium
  - Shape
  - Packing
- Larger parameter space
- Access metastable crystal states
- Useful for:
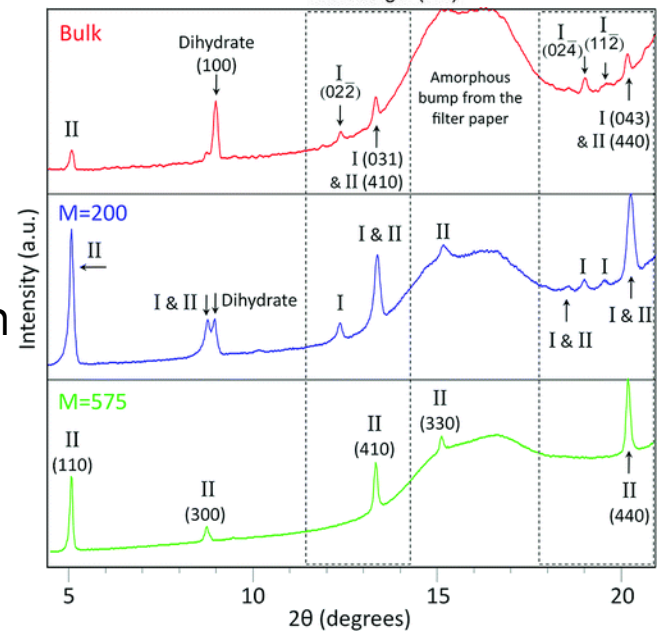 - OSCs
  - Biopharma
  - Food processing
  - Photonics

Liu et al
Langmuir 2011

BCC → FCC
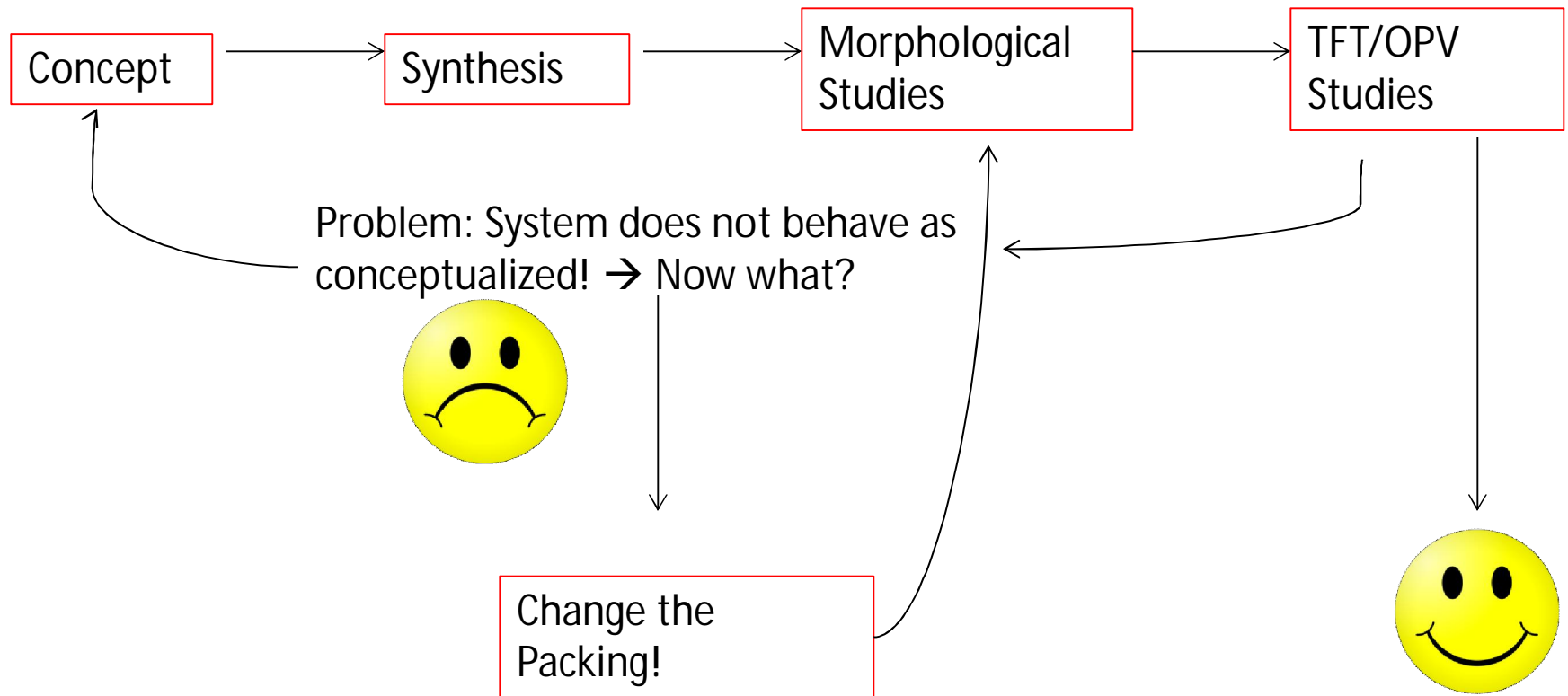
Drug polymorph control

Diao et. al. JACS 2012

Kinetic Crystallization for OSCs

- Want high mobility, high performance
- Normal Step:

| Concept | Synthesis | Morphological Studies | TFT/OPV Studies |

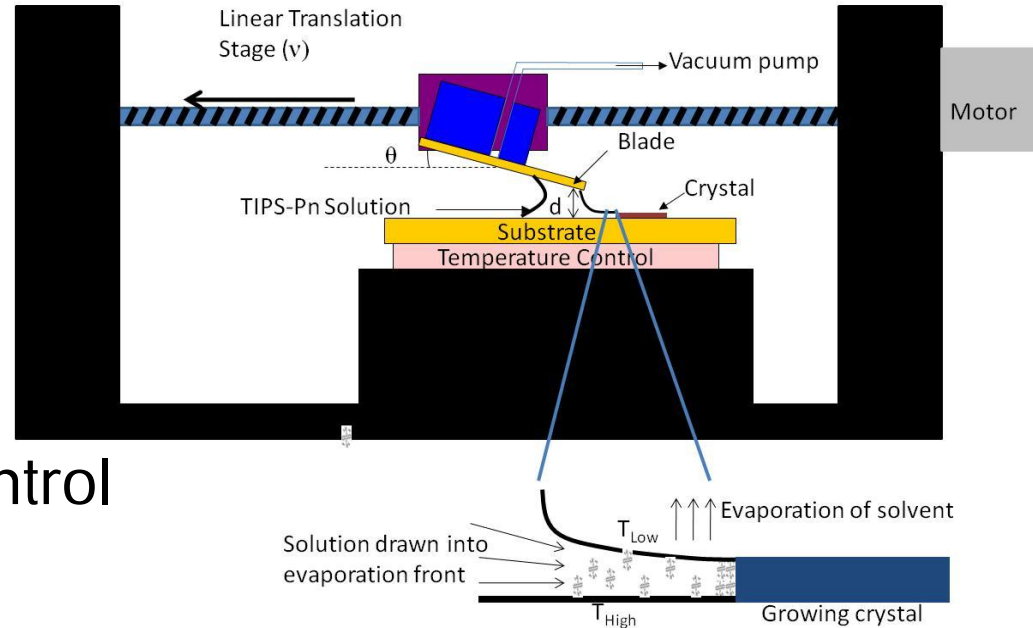Problem: System does not behave as conceptualized! → Now what?

Change the Packing!

Advantage: A shortcut!
Disadvantage: Larger parameter space

Solution Shearing Method (SSM)

- Use evaporation front
  - Front alone exposed to ambient
  - Continuous processing
  - Uniform film deposition
  - Crystallization speed control
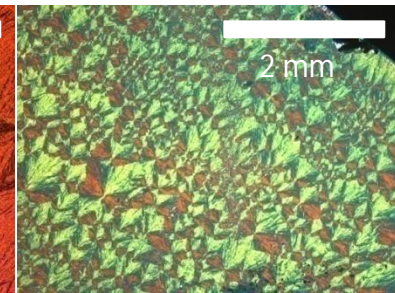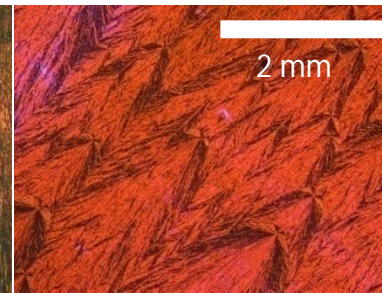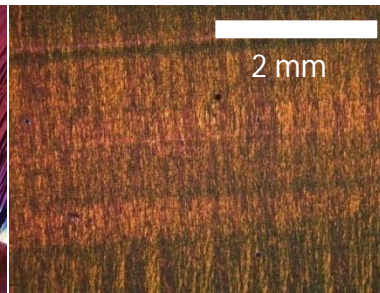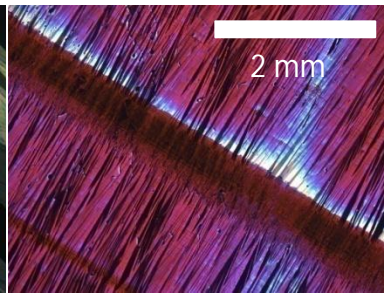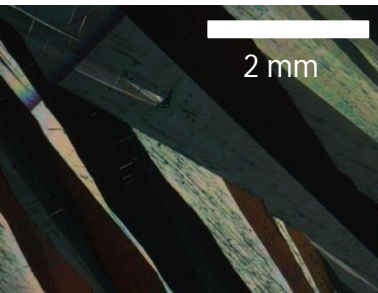- Can modify crystal morphology and packing

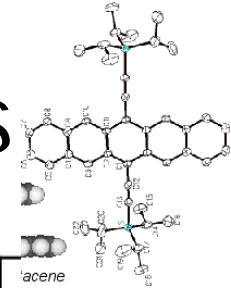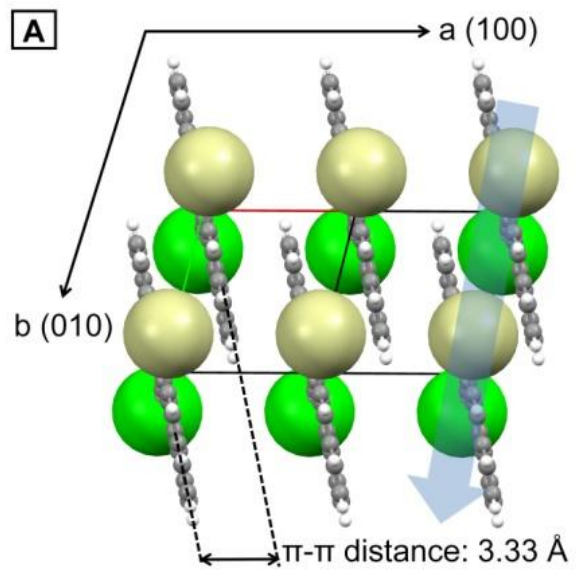| 0.4 mm/s	1.6 mm/s	2.8 mm/s	4 mm/s	8 mm/s

GIXD and Strain
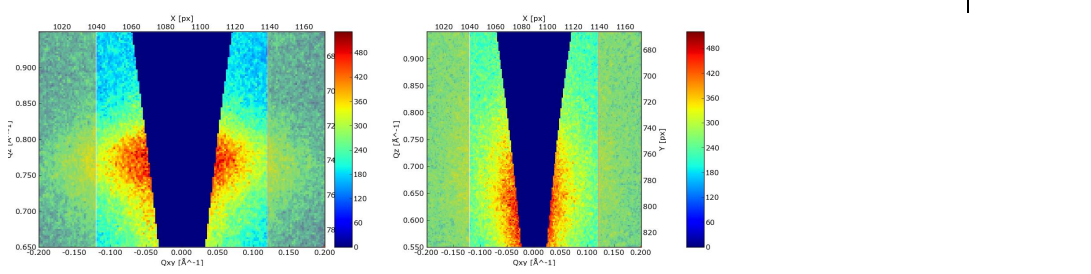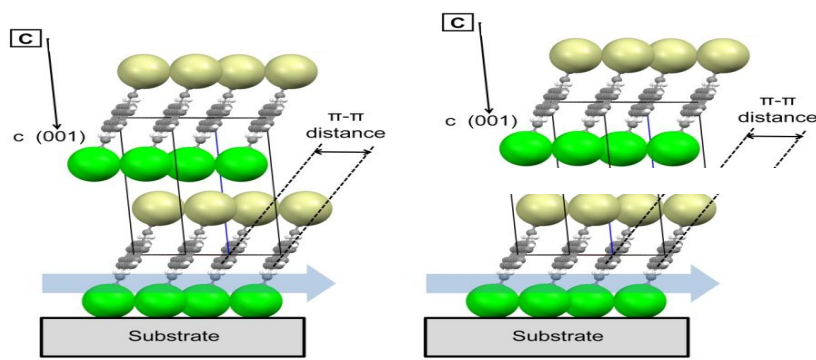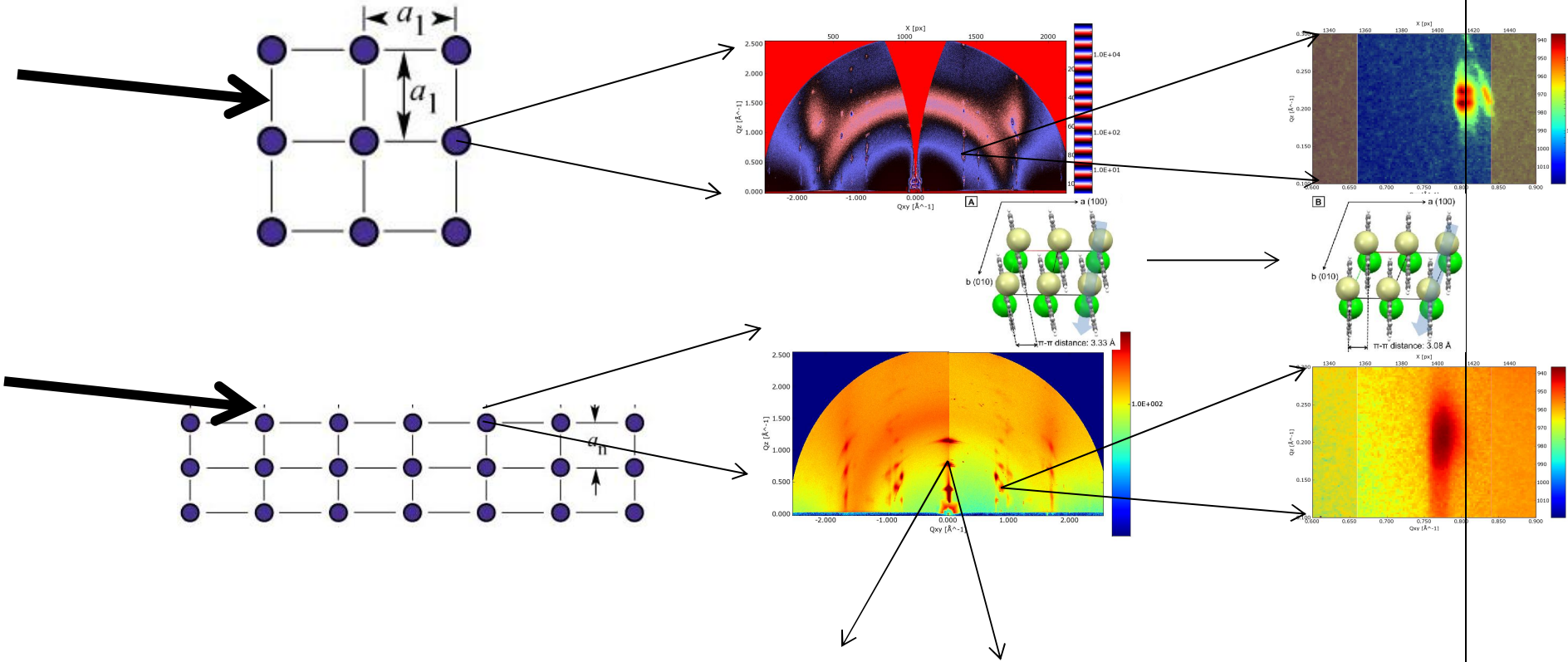
Strain of 2D Brick-wall Packing Systems TIPS-Pr

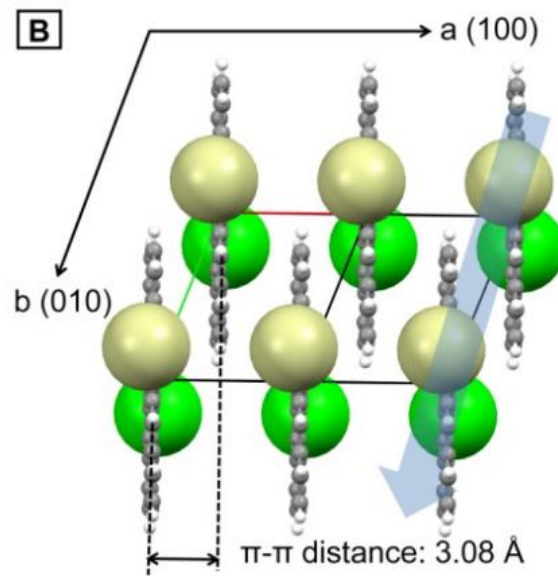- Can see packing shift
- Cell becomes oblique, in plane shift
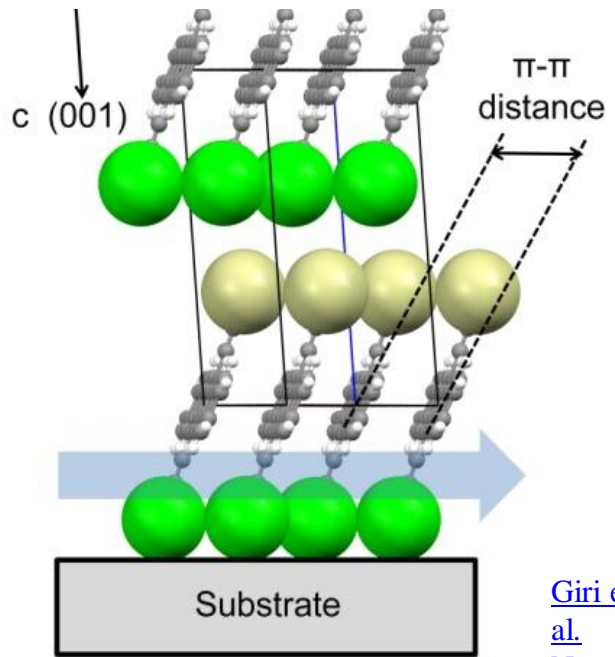
- Changes π-π stacking dist.
- Explains higher mobility

Molecular Pair	t (meV)	Center-of-mass distance (A)
Evaporated thin film (01)	11.7	7.832
Evaporated thin film (02)	-2.32	10.083
Thin film sheared at 8 mm/s (01)	-36.9	8.560
Thin film sheared at 8 mm/s (02)	-0.429	9.512

A → a (100)

b (010)

π-π distance: 3.33 Å

Evaporated

B → a (100)

b (010)

π-π distance: 3.08 Å

Sheared 8mm/s

c (001)

π-π distance

Substrate

Sheared

Giri et al. Nature 2012