

DTU



Model Supported in-line Characterization of Roll-to-Roll Coated Organic Solar Cells

The 23rd Sede Boqer Symposium on Solar Electricity Production
September 5-7, 2022

Ben-Gurion University of the Negev

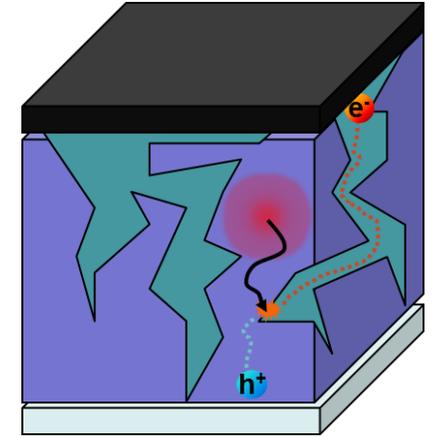
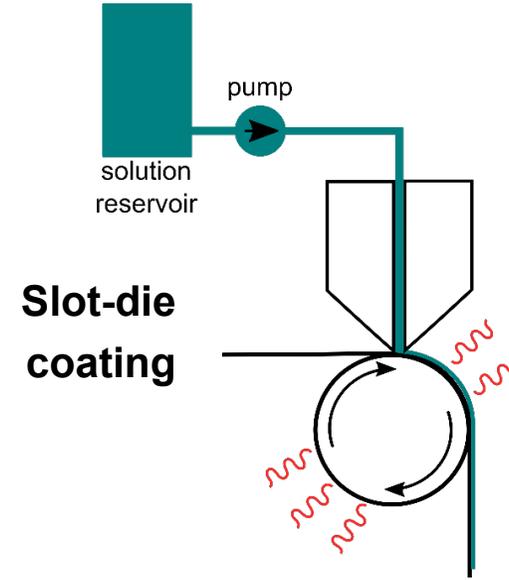
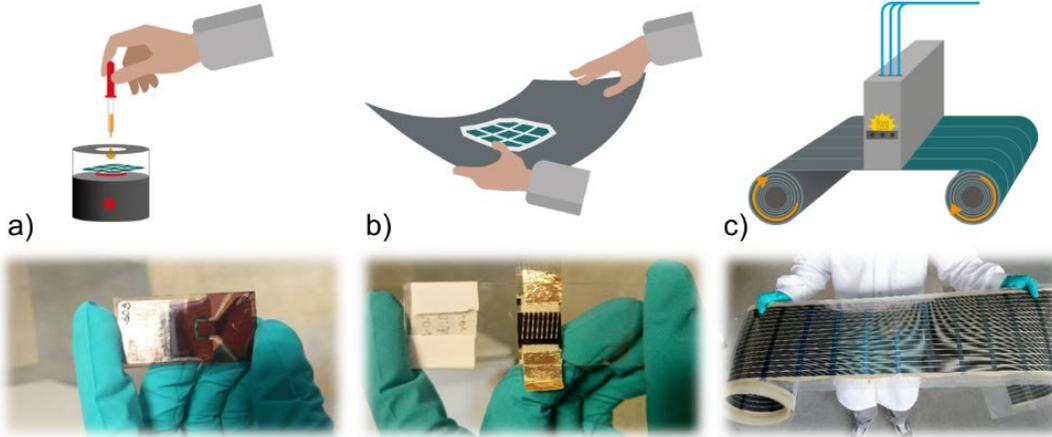
[Jens Wenzel Andreasen, jewa@dtu.dk](mailto:jewa@dtu.dk)

From lab-to-fab: towards scalability

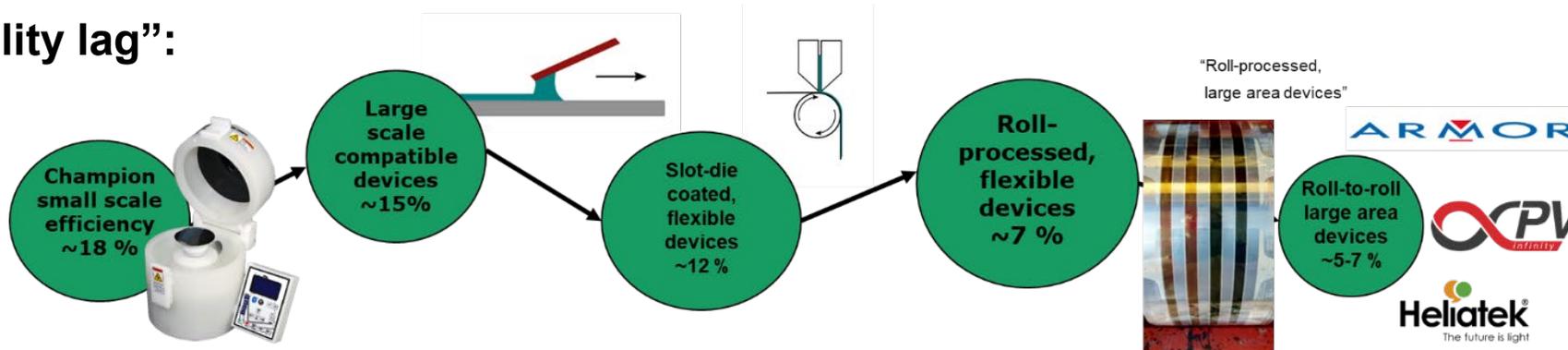
LAB

to

FAB

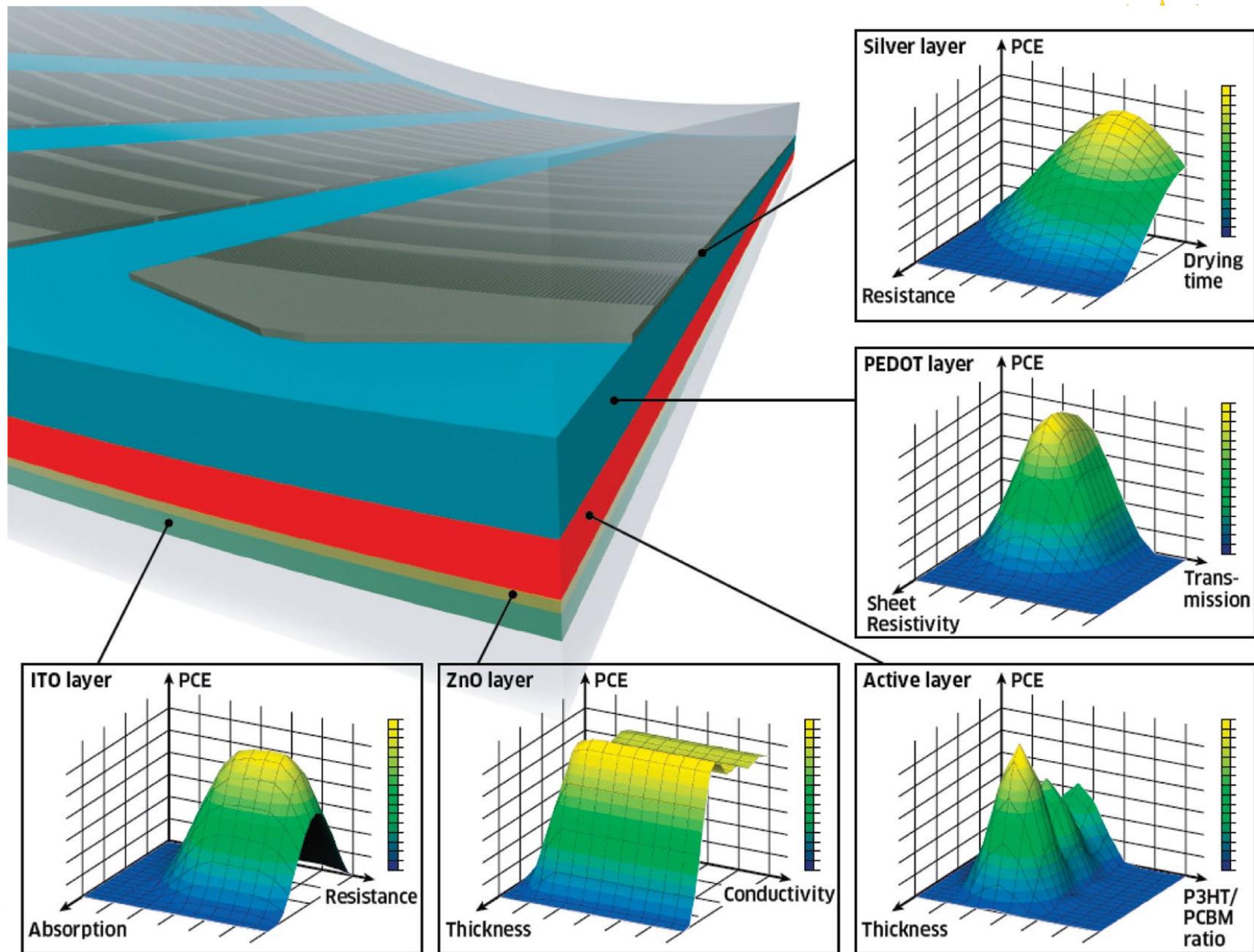


“Scalability lag”:



Optimization:

Tedious, slow, requires a lot of material



Jan Alstrup, Mikkel Jørgensen, Andrew J. Medford, and Frederik C. Krebs, *Ultra Fast and Parsimonious Materials Screening for Polymer Solar Cells Using Differentially Pumped Slot-Die Coating*, ACS Appl. Mater. Interfaces 2010, **2**, 10, 2819-2827

Optimization:

Tedious, slow, requires a lot of material

Solution:

Leverage the potential of high-throughput, fine-grained testing of the R2R platform

Jan Alstrup, Mikkel Jørgensen, Andrew J. Medford, and Frederik C. Krebs, *Ultra Fast and Parsimonious Materials Screening for Polymer Solar Cells Using Differentially Pumped Slot-Die Coating*, ACS Appl. Mater. Interfaces 2010, 2, 10, 2819-2827

Conventional device on glass study

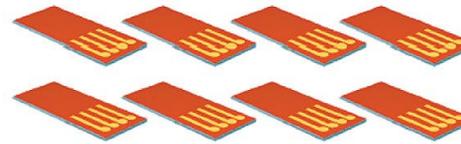
1. Prepare solutions



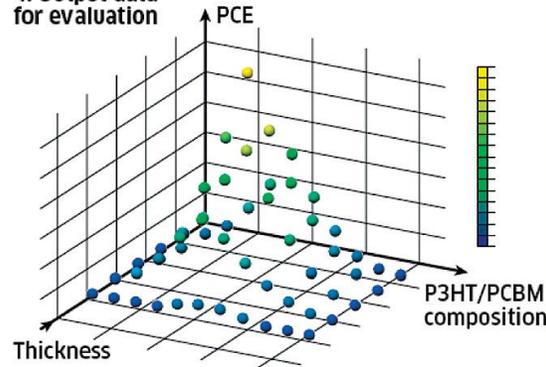
2. Manual device preparation by spin coating



3. Individual device characterization

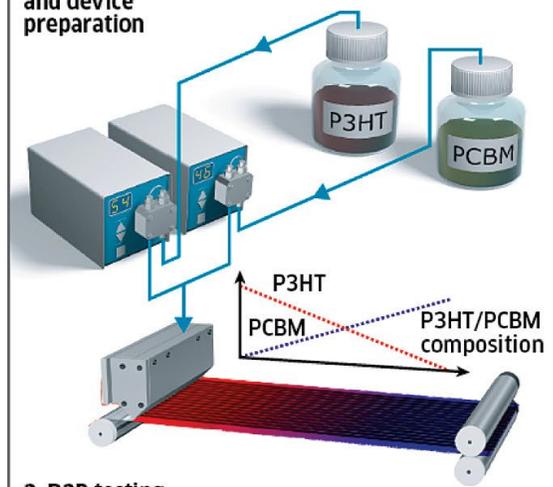


4. Output data for evaluation



R2R study

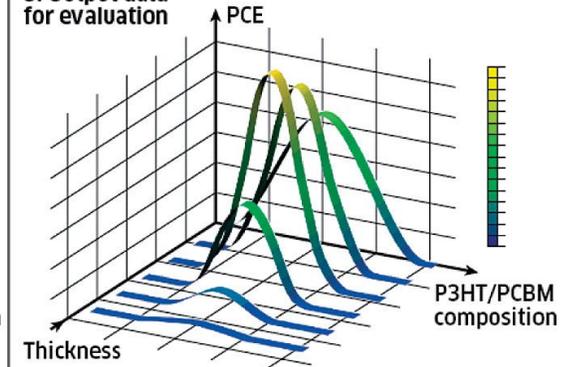
1. Continuous mixing and device preparation



2. R2R testing

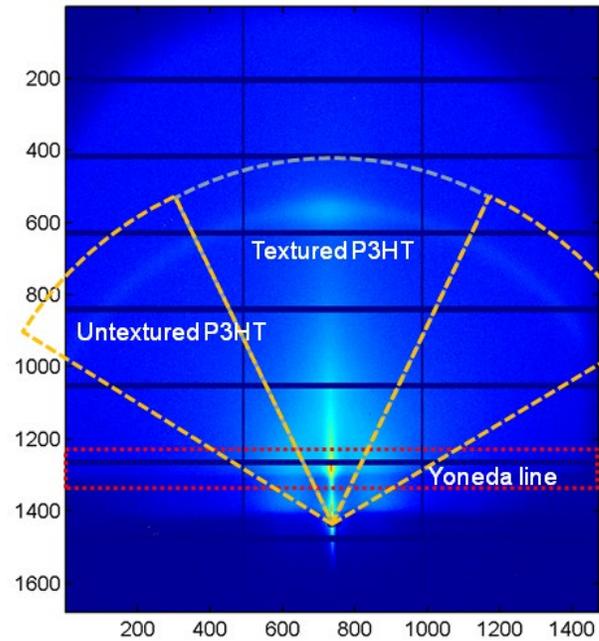


3. Output data for evaluation

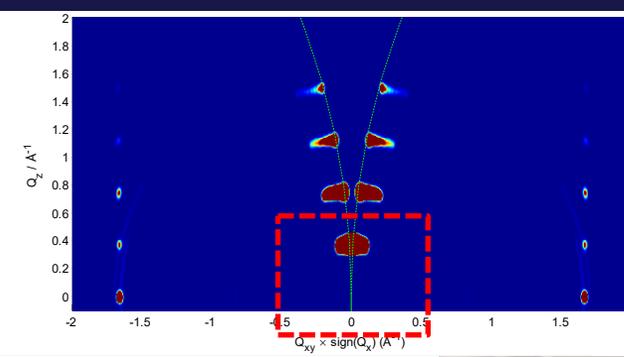
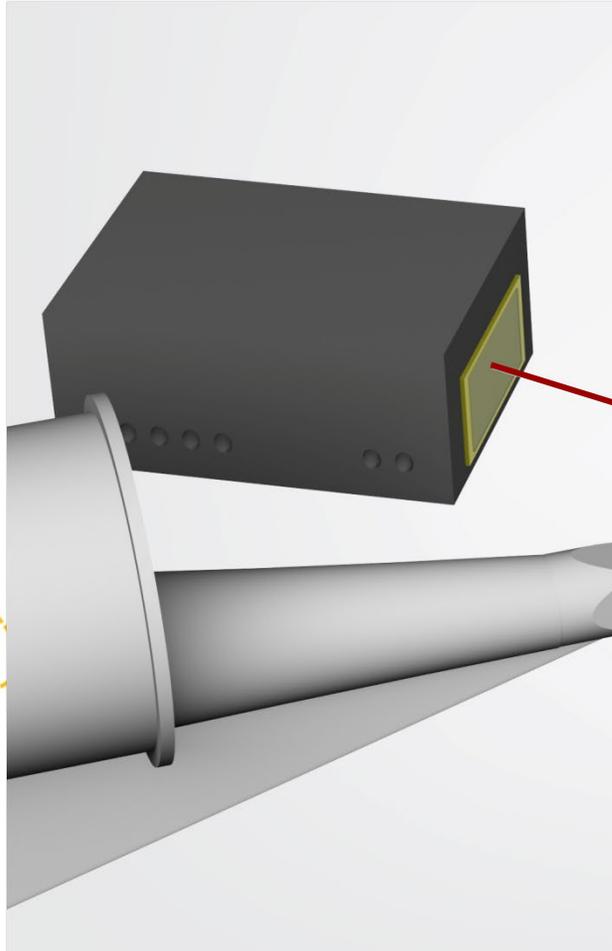


GIWAXS = Grazing Incidence Wide Angle X-ray Scattering

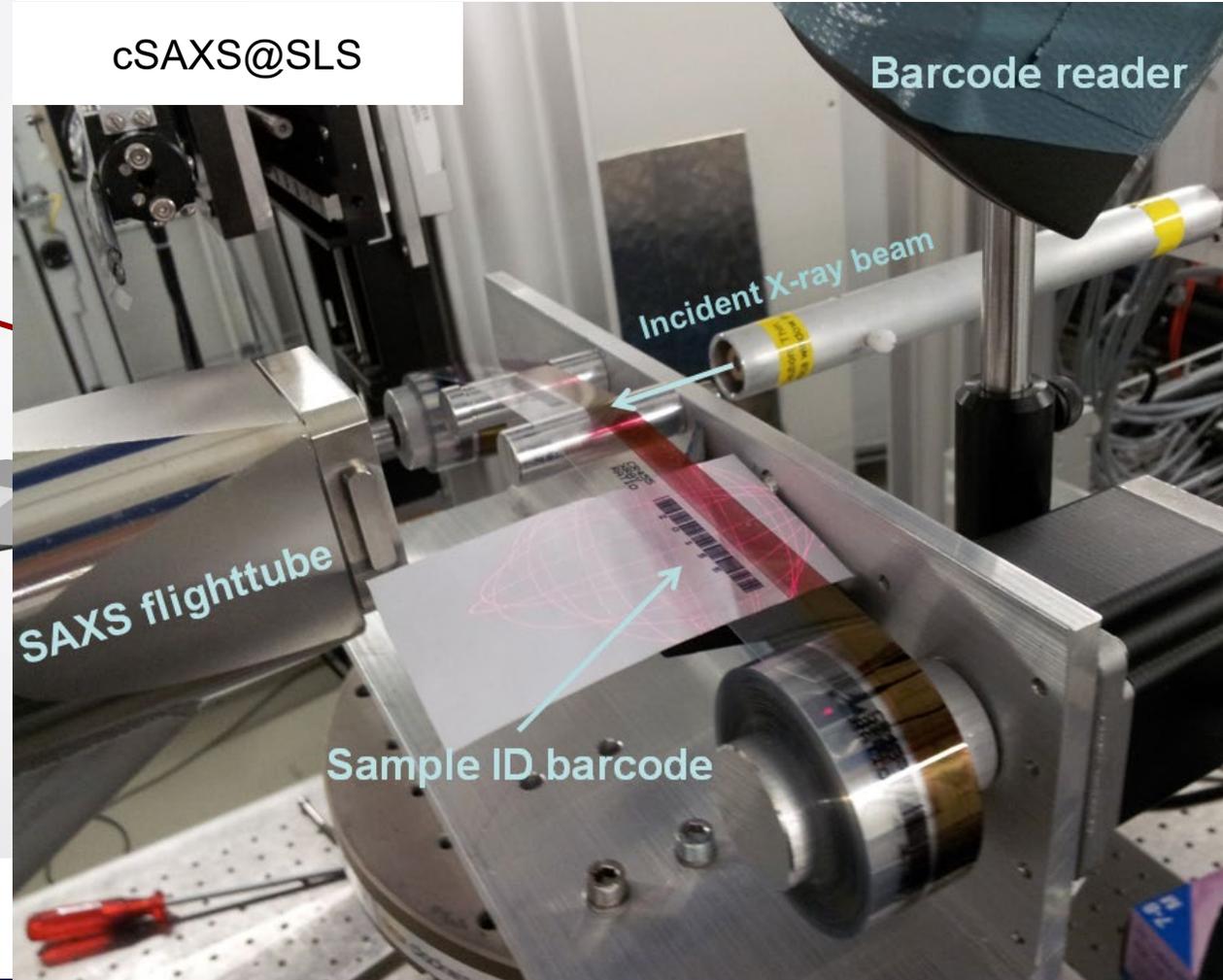
Arvid P. L. Böttiger, Mikkel Jørgensen, Andreas Menzel, Frederik C. Krebs and Jens W. Andreasen, *High-throughput roll-to-roll X-ray characterization of polymer solar cell active layers*, J. Mater. Chem., 2012 **22**, 22501-22509



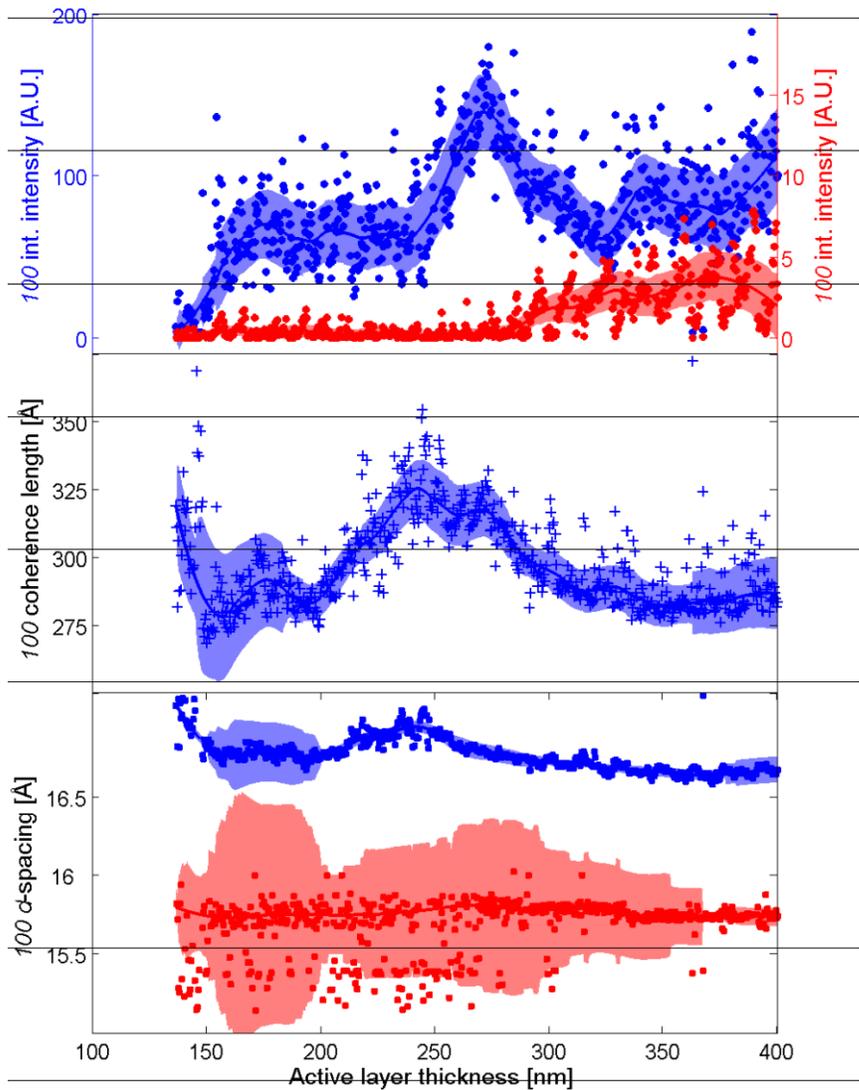
GISAXS = Grazing Incidence Small X-ray Scattering



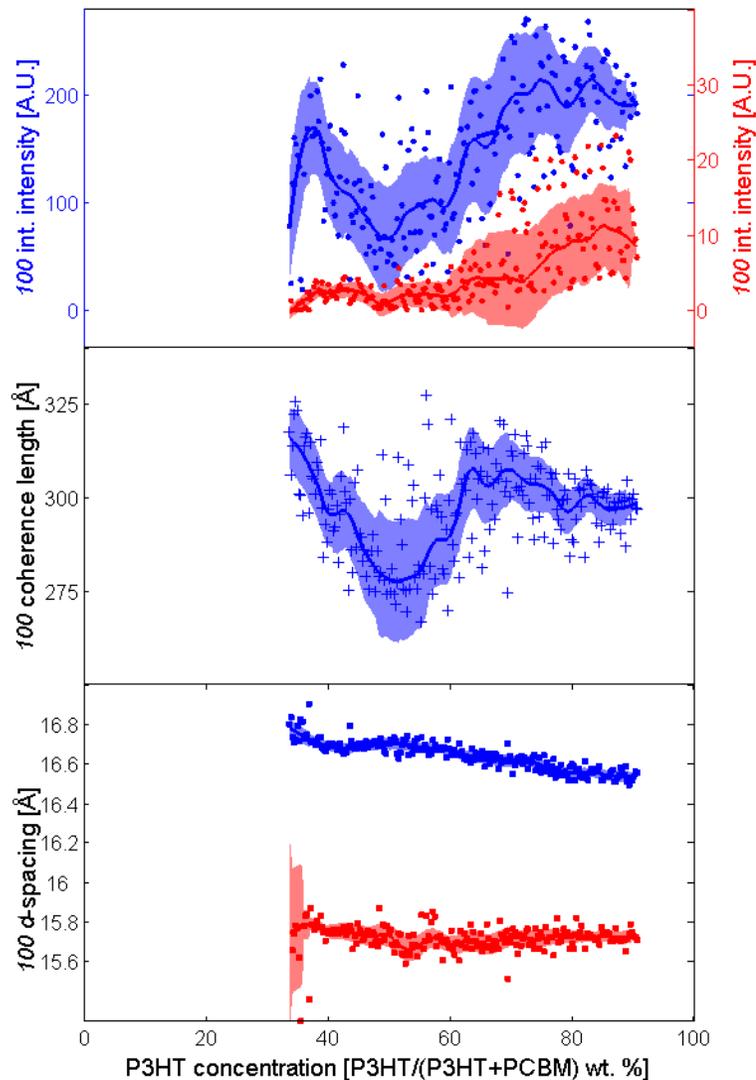
cSAXS@SLS



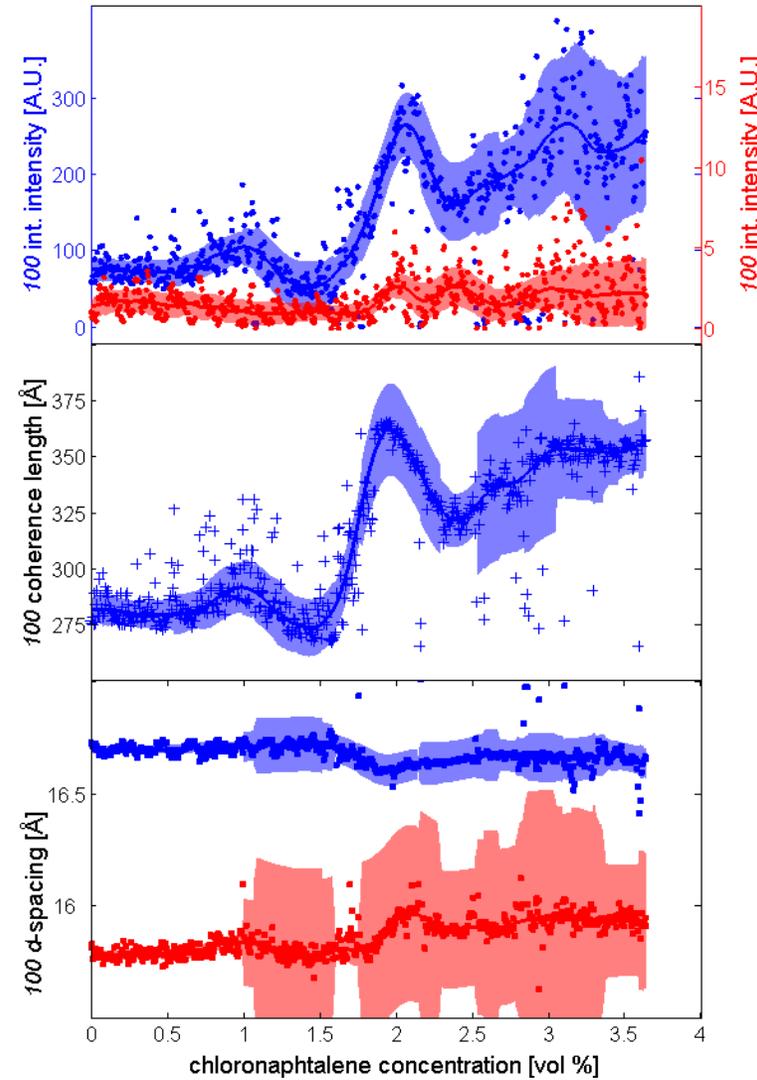
Thickness gradient P3HT:PCBM 1:1



Ratio gradient P3HT:PCBM

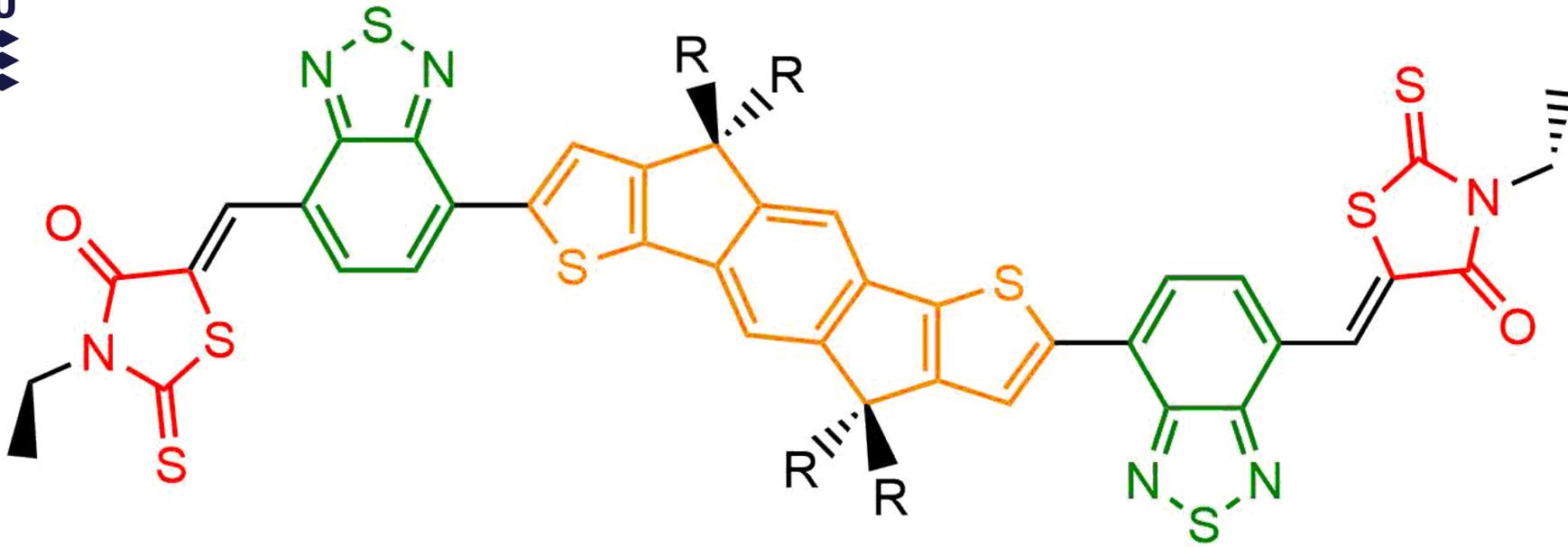


additive gradient chloronaphtalene



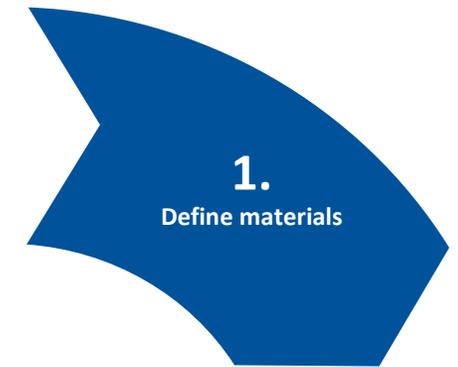
But, really this is also trial and error, just faster. Can we do something better...?





EH-IDTBR: R = 2-ethylhexyl

O-IDTBR: R = octyl



- **O-IDTBR** -> complementary absorption to P3HT

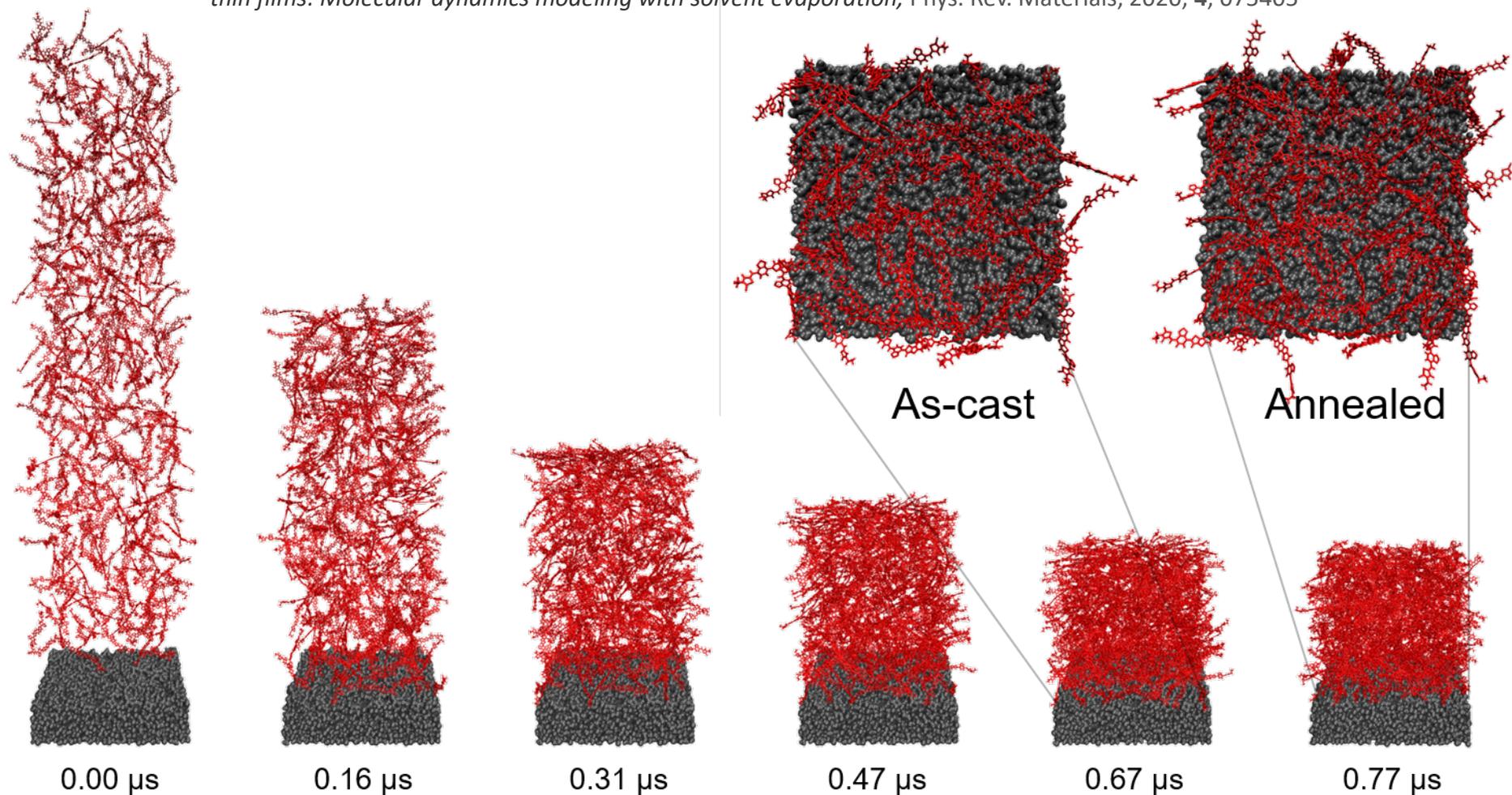
- **P3HT:O-IDTBR:**

- High industrial figure of merit (i-FoM)*

$$i - FoM = \frac{PCE \times Stability}{SC_{index}}$$

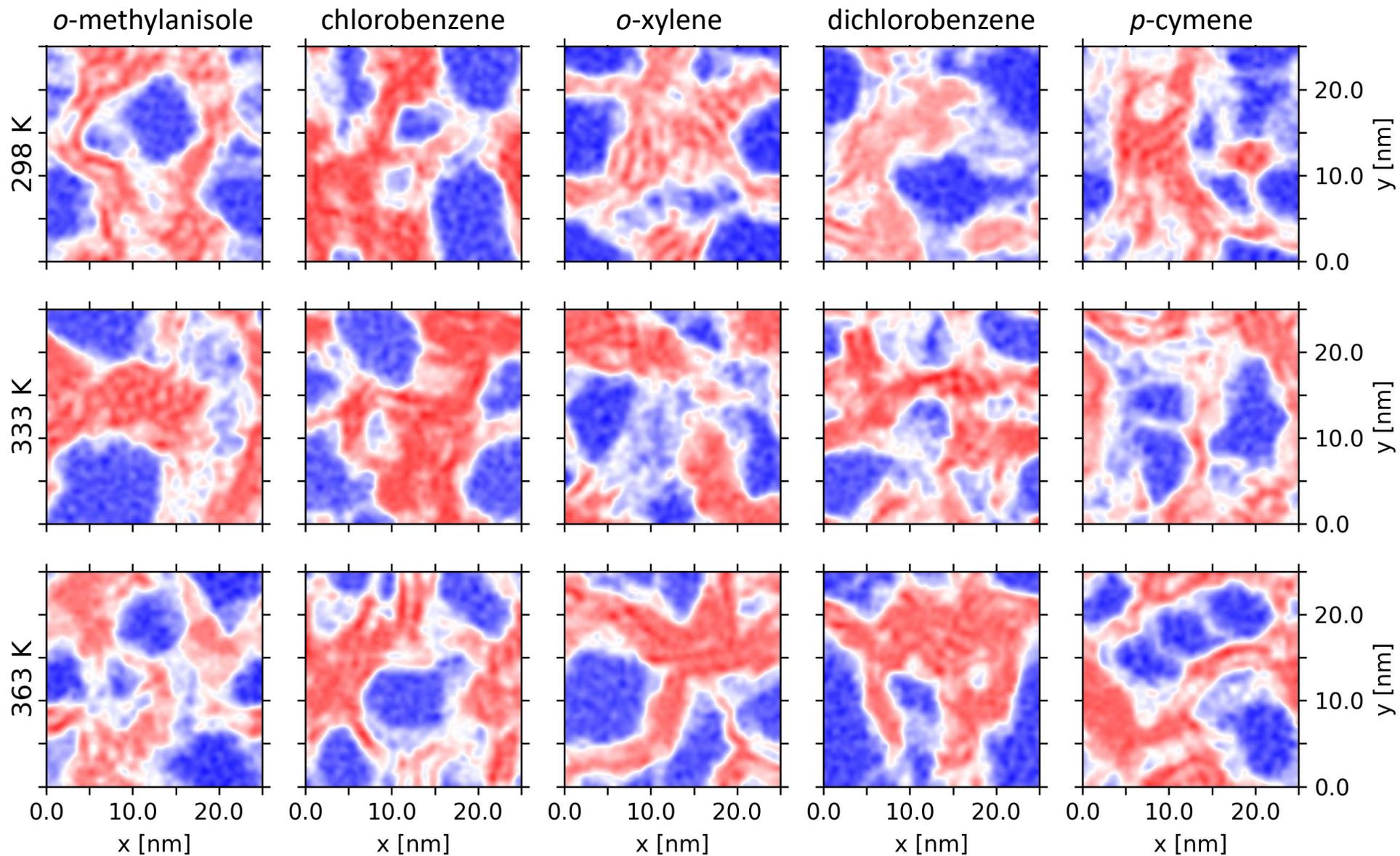
- Efficiencies above 7% in lab-scale
- Low scalability-lag in previous studies

*Adv. Energy Mater. 2017, 7, 1700465.

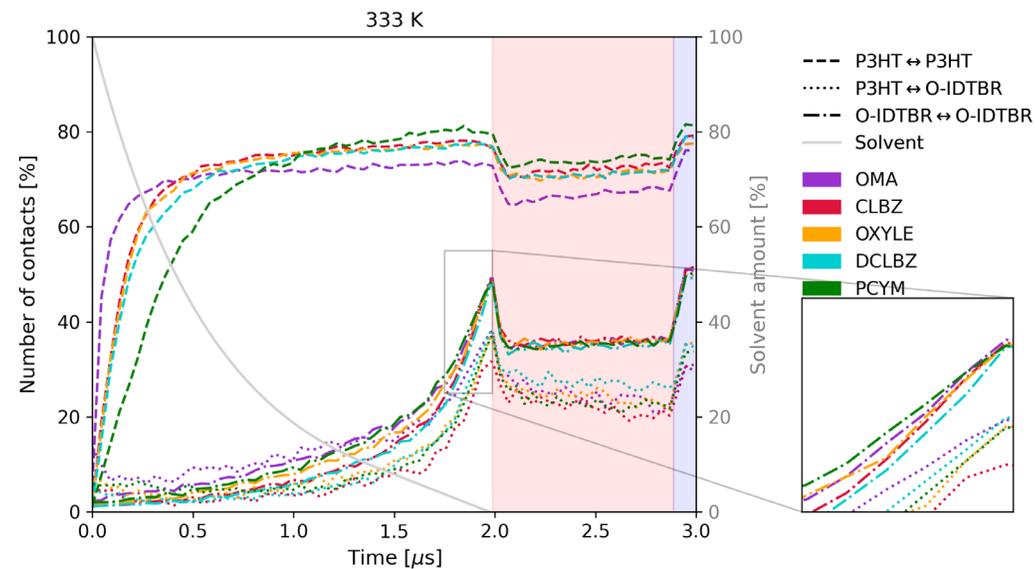
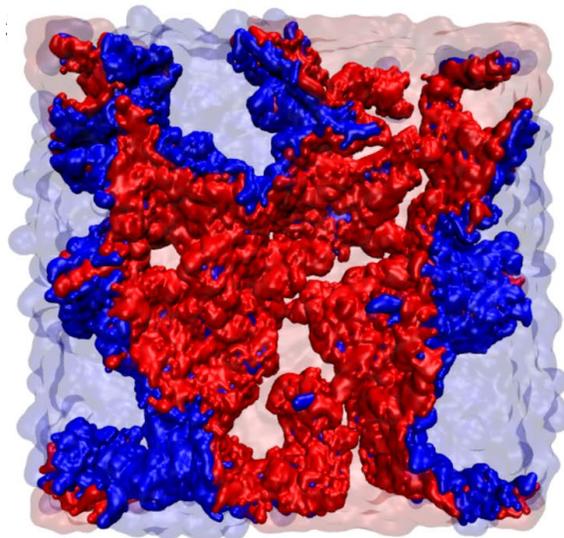


2. Predict
structure by
MD

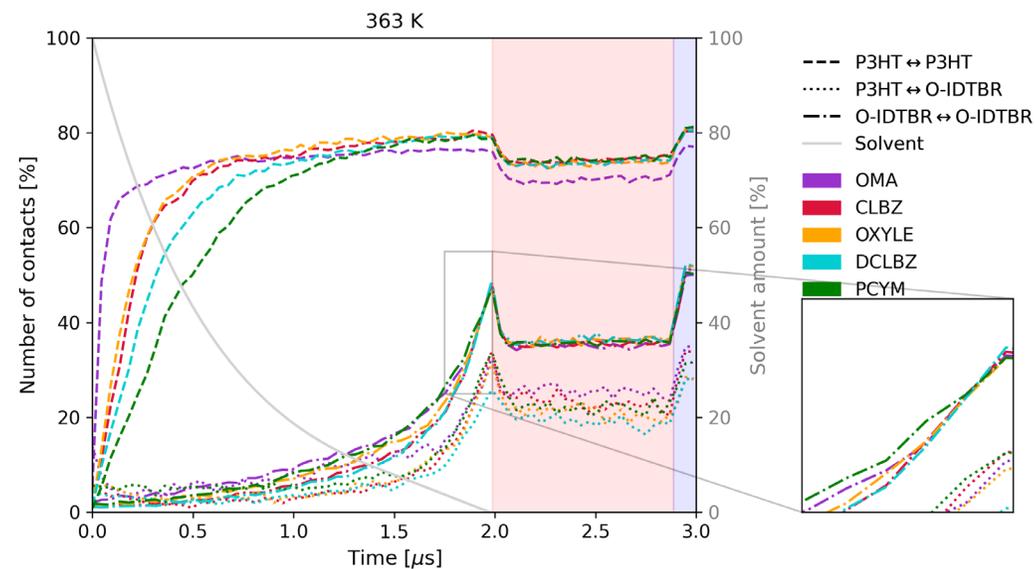
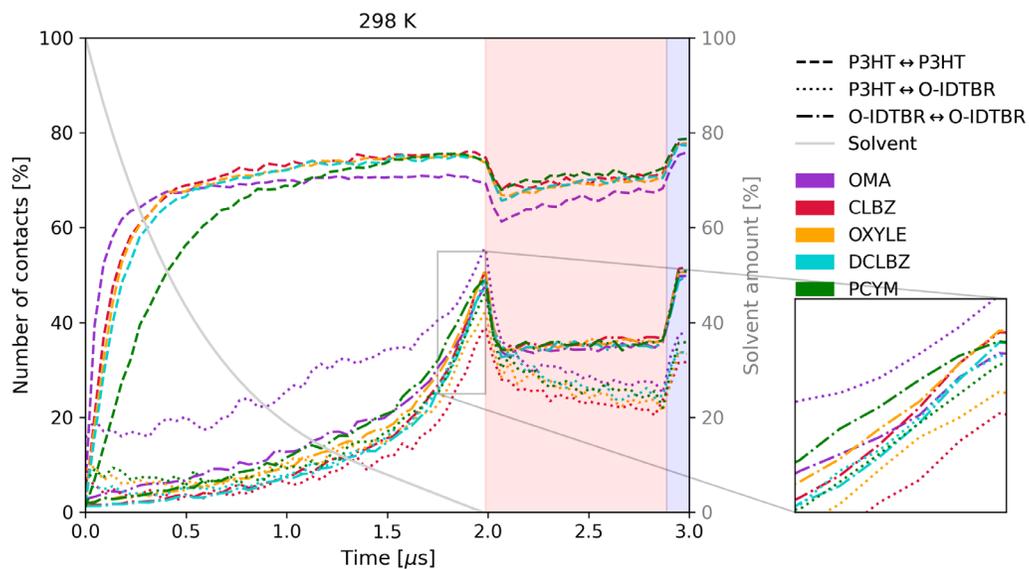
Visualization of the solvent evaporation procedure for O-IDTBR (red) on an amorphous SiO₂ substrate (gray). The final frames from five steps out of the total 133 steps are shown in addition to the annealed thin-film with their corresponding simulation times. Insets show the bottom layer of IDTBR molecules, i.e., molecules that are fully or partly within 4.5 Å of the substrate, for the as-cast and annealed thin-films. Side chains and solvent molecules are not shown for clarity.

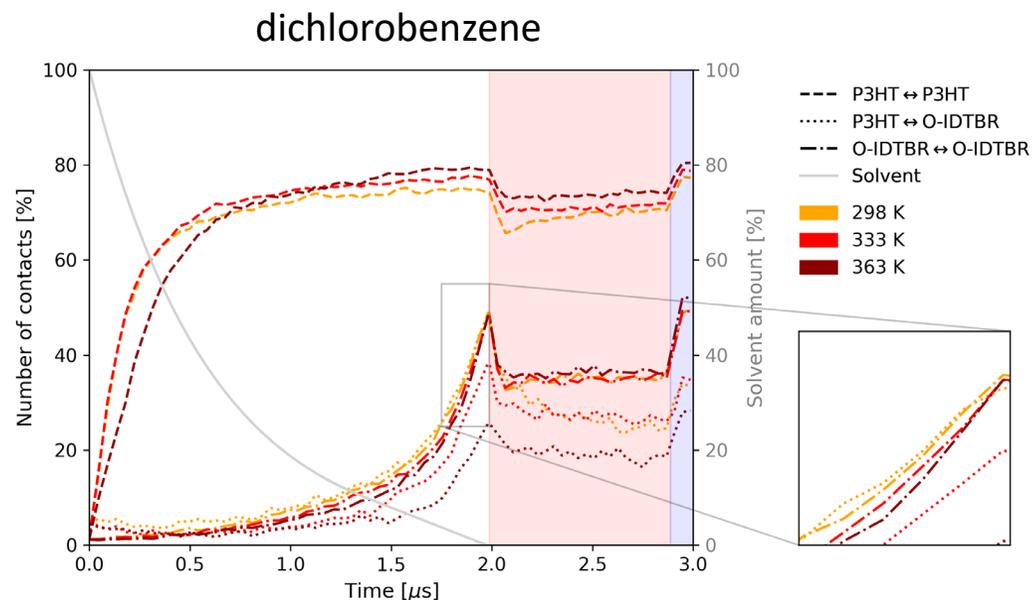
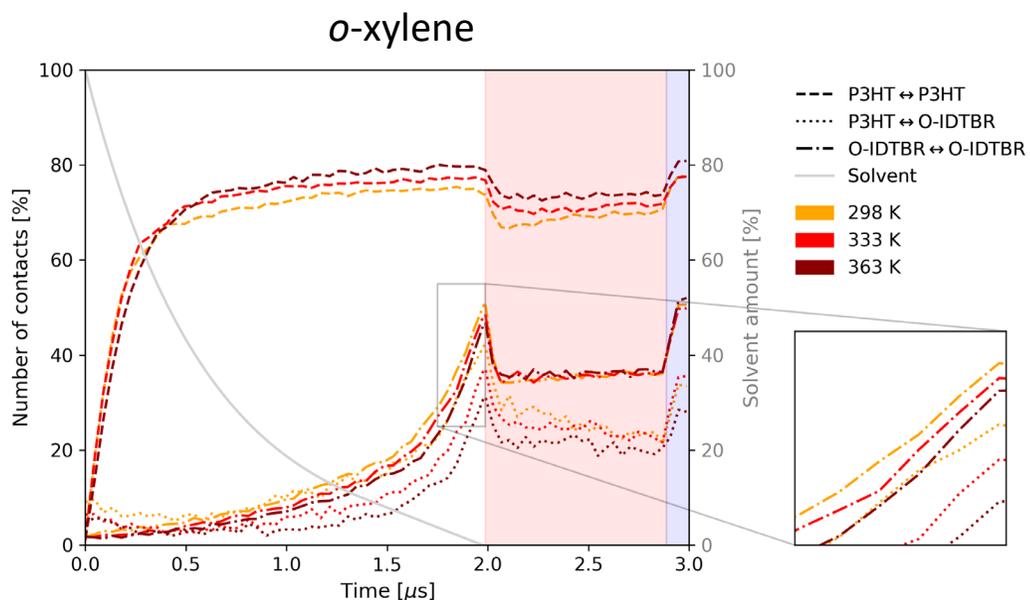
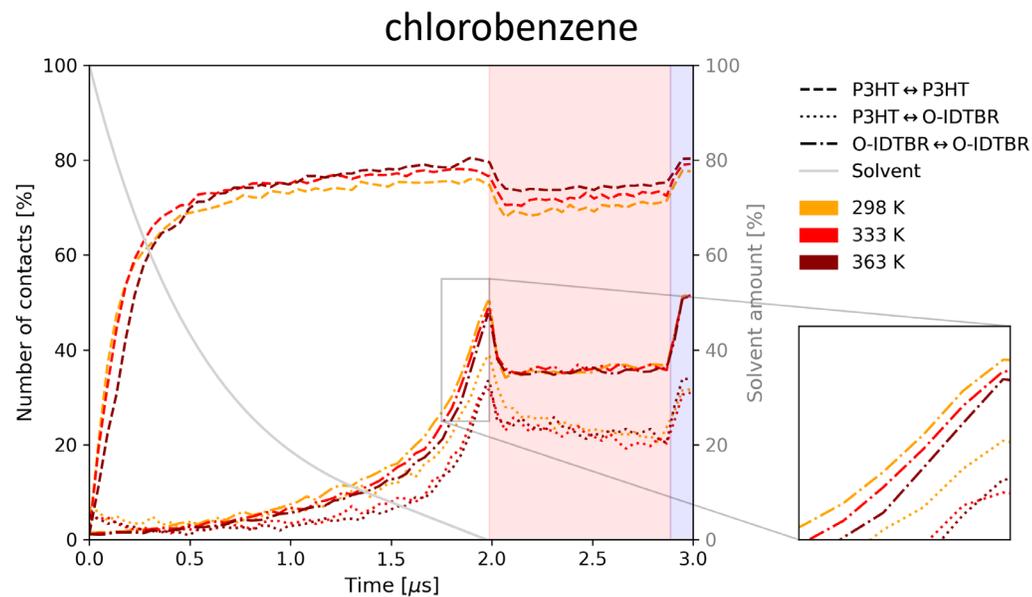
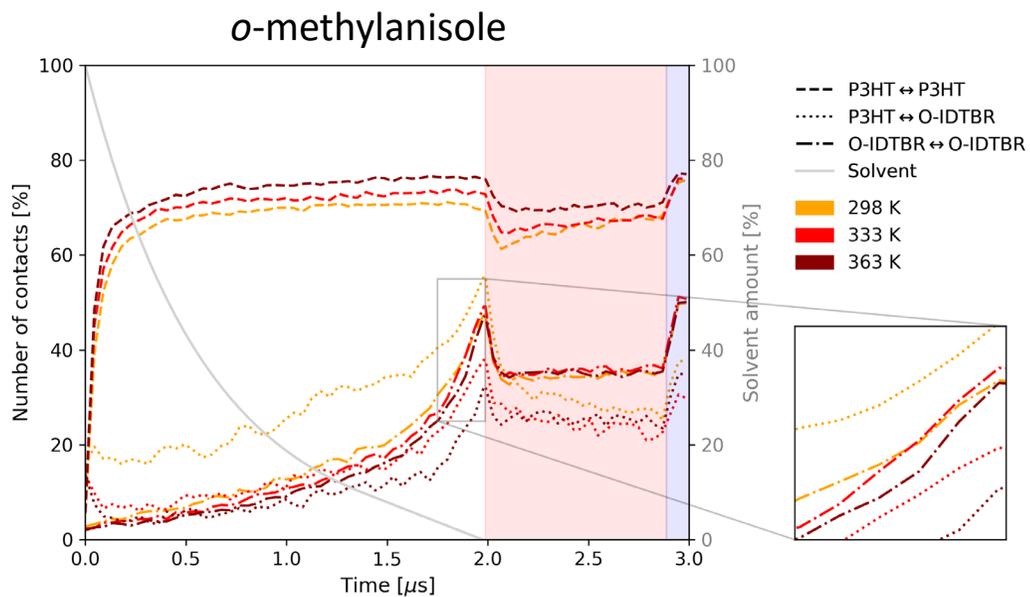


2. Predict structure by MD



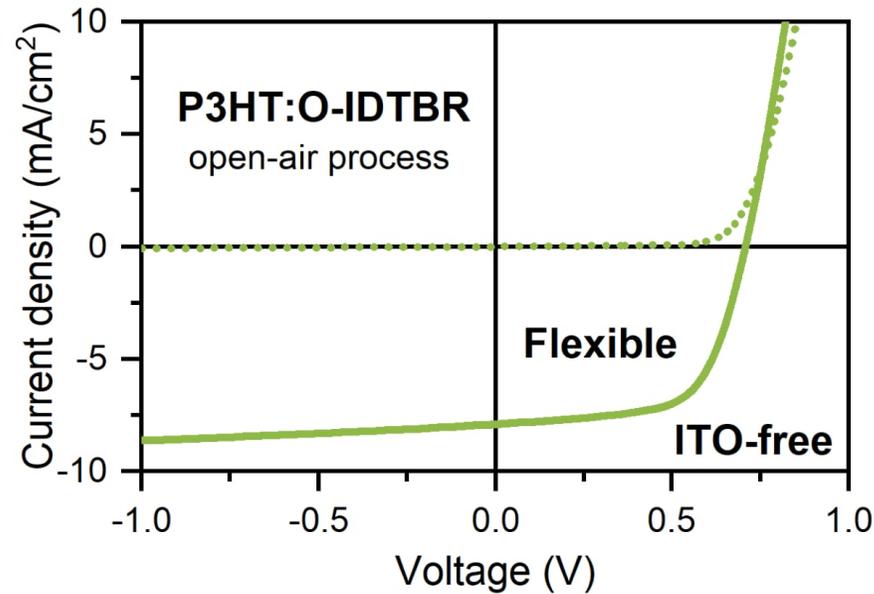
2. Predict structure by MD





2. Predict structure by MD

Solar cell devices



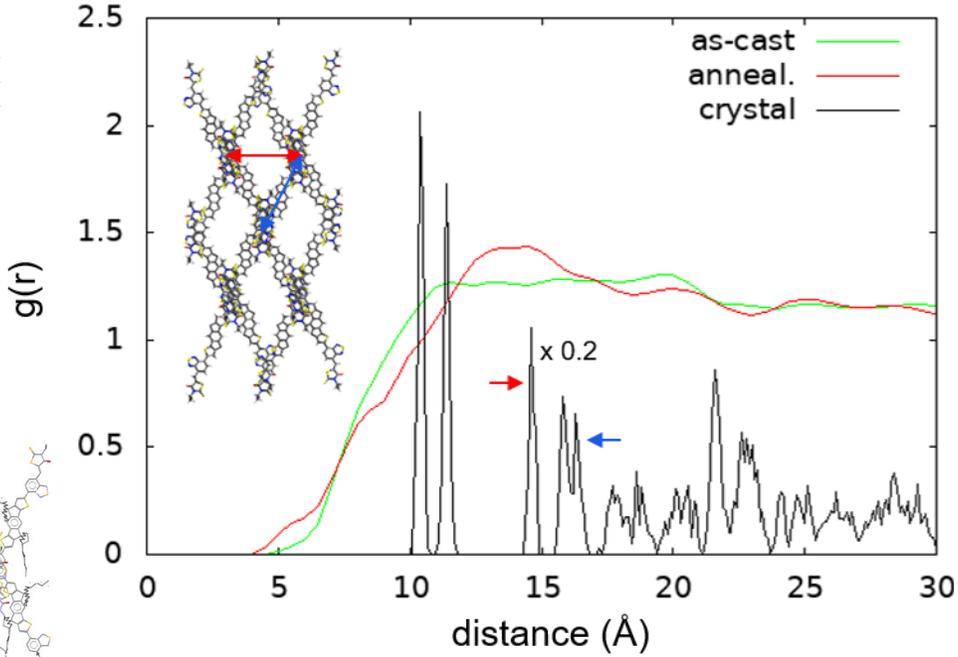
PCE = 3.59%
 FF = 64.27%
 $J_{SC} = 7.90 \text{ mA/cm}^2$
 $V_{OC} = 0.71 \text{ V}$
 $R_S = 6.10 \text{ } \Omega/\text{cm}^2$
 $R_{Sh} = 1.03 \text{ k}\Omega/\text{cm}^2$
 Area = 1 cm²

- An optimization approach to upscale NFA-based OSCs to slot-die coating in a roll-processing was successfully applied. It can be used as a general approach.
- P3HT:O-IDTBR is a suitable candidate for upscaling. Short EPBTs.
- Efficiencies up to **3.6%** for **fully printed devices (1 cm²)**
- Ag performs as the best candidate for the back electrode, followed by Cu (cost reduction)
- Larger area devices (up to 4 cm²) were fabricated. Homogeneous stripe.

3. Make the devices

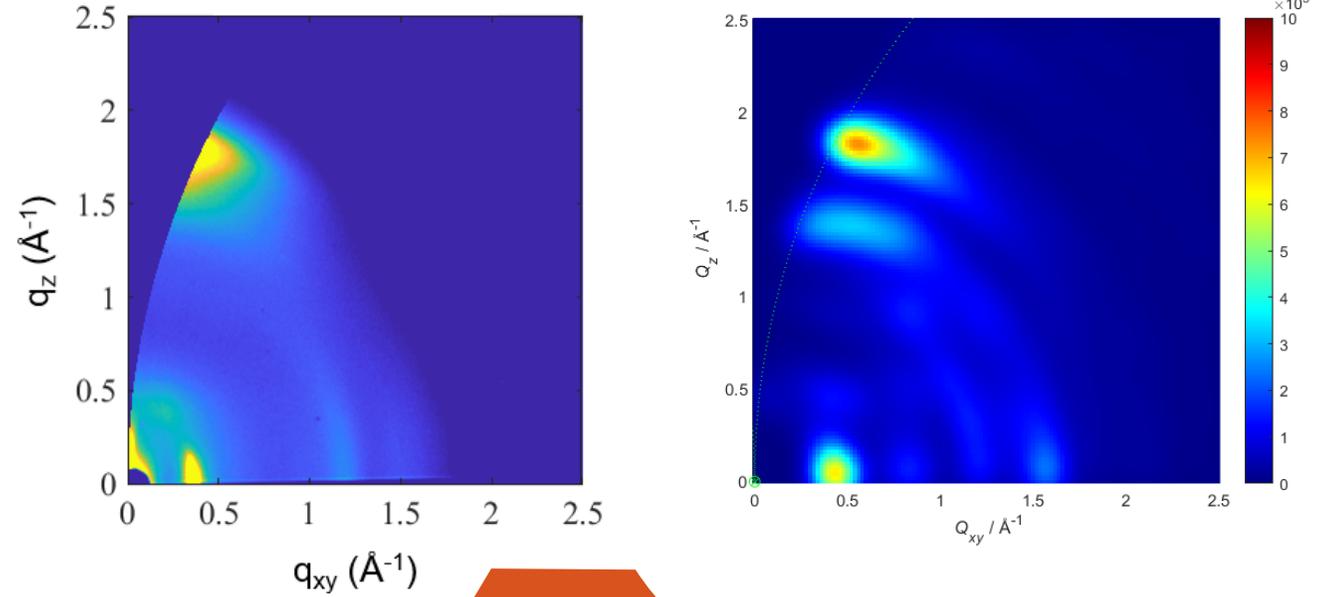
M. Fernández Castro, E. Mazzolini, R. R. Sondergaard, M. Espindola-Rodriguez, and J. W. Andreasen, *Flexible ITO-Free Roll-Processed Large-Area Nonfullerene Organic Solar Cells Based on P3HT:O-IDTBR*, Phys. Rev. Appl. **14**, 034067 (2020).

O-IDTBR



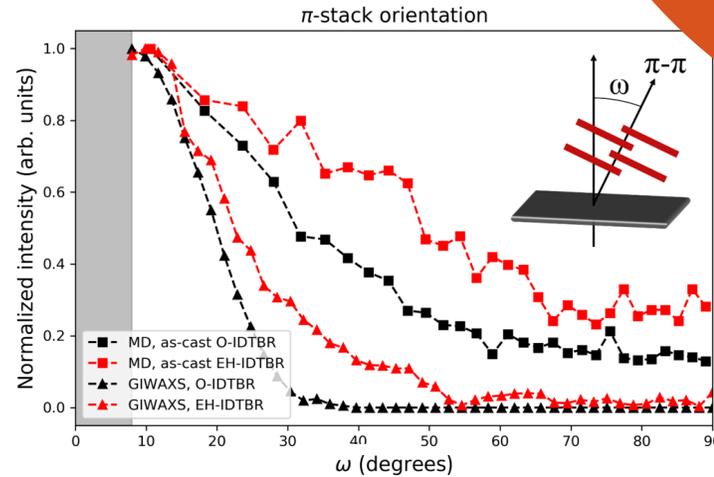
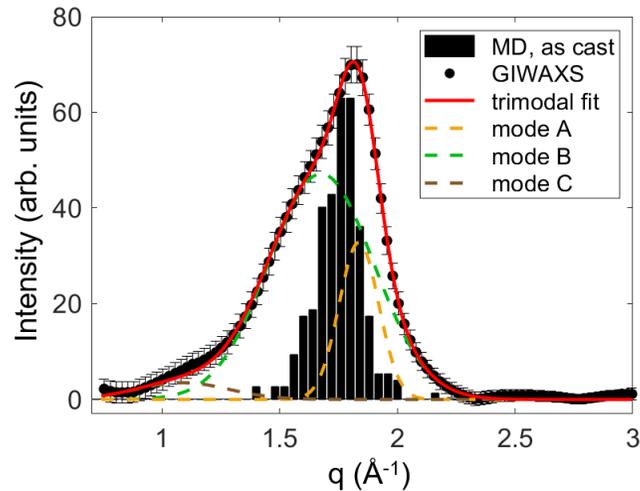
Bristow et al. *Advanced Electronic Materials*, 2019, 1900344

O-IDTBR 70°C

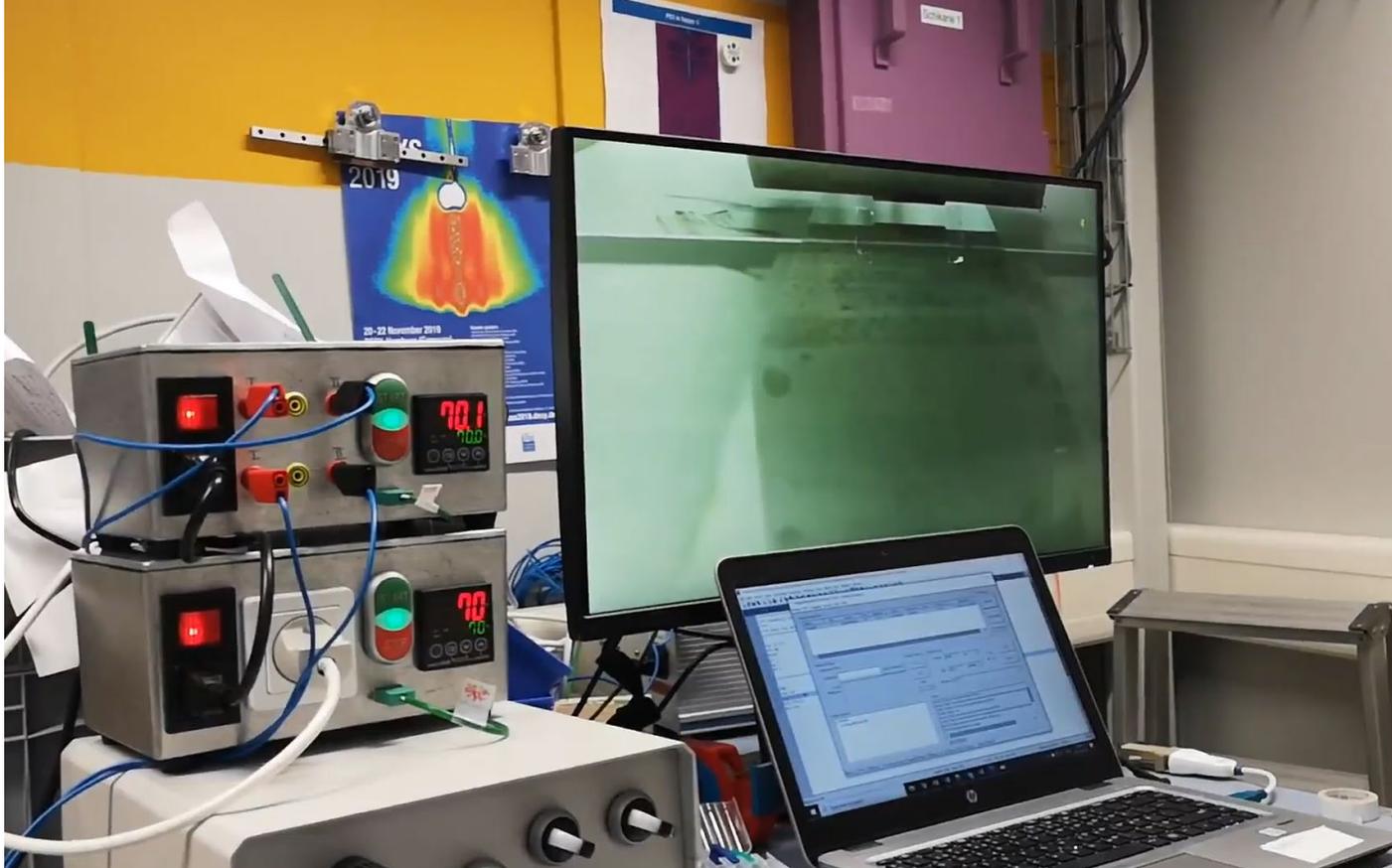


4.

Validate structure



Anders S. Gertsen, Michael Korning Sørensen, and Jens W. Andreasen, *Nanostructure of organic semiconductor thin films: Molecular dynamics modeling with solvent evaporation*, *Phys. Rev. Materials*, 2020, **4**, 075405



P03@PETRAIII DESY Hamburg

4.

Validate structure

***in situ* X-ray scattering during hot-hot-hot roll-2-roll coating**



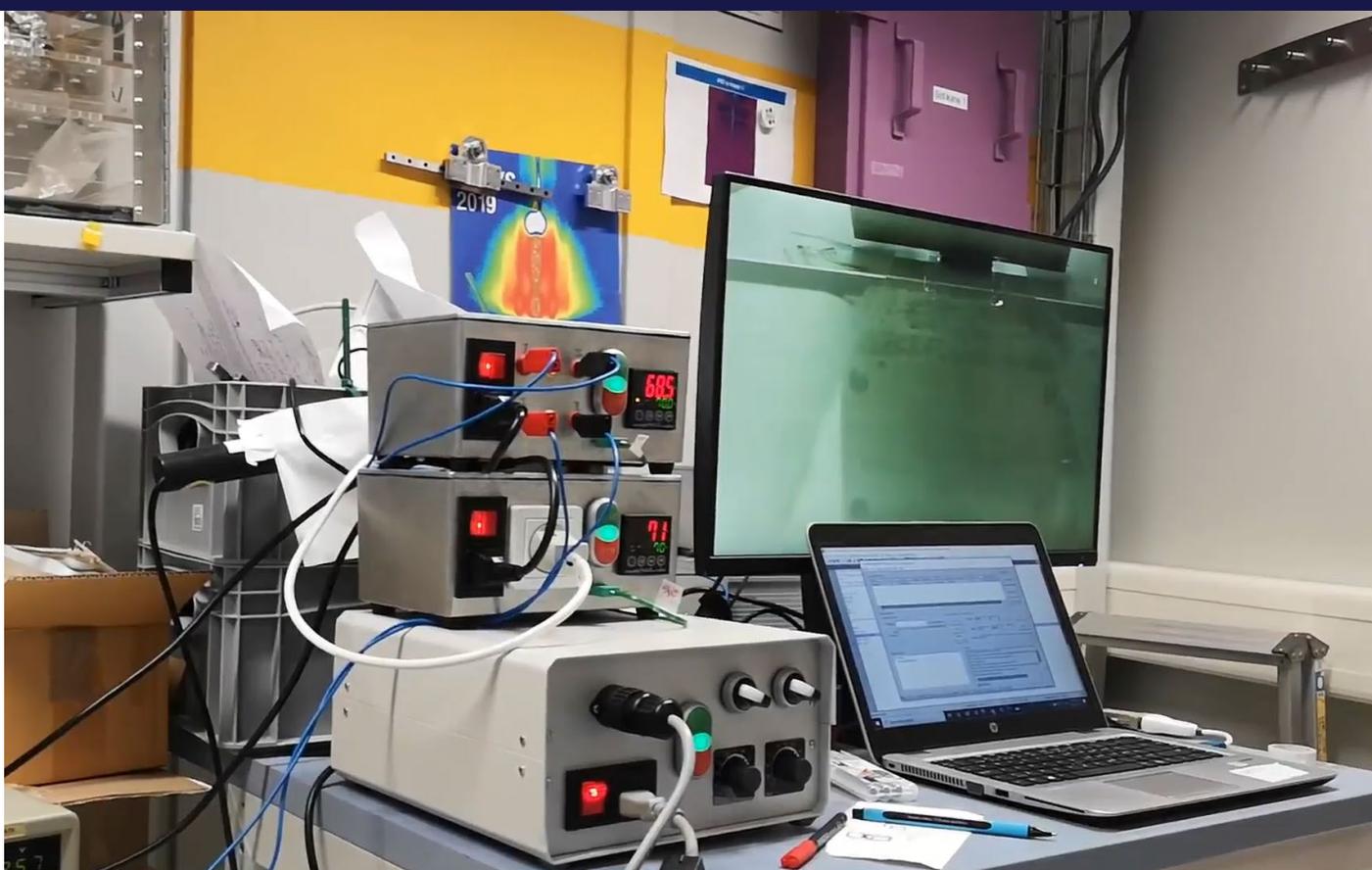
P03@PETRAIII DESY Hamburg

4.

Validate structure

***in situ* X-ray scattering during hot-hot-hot roll-2-roll coating**

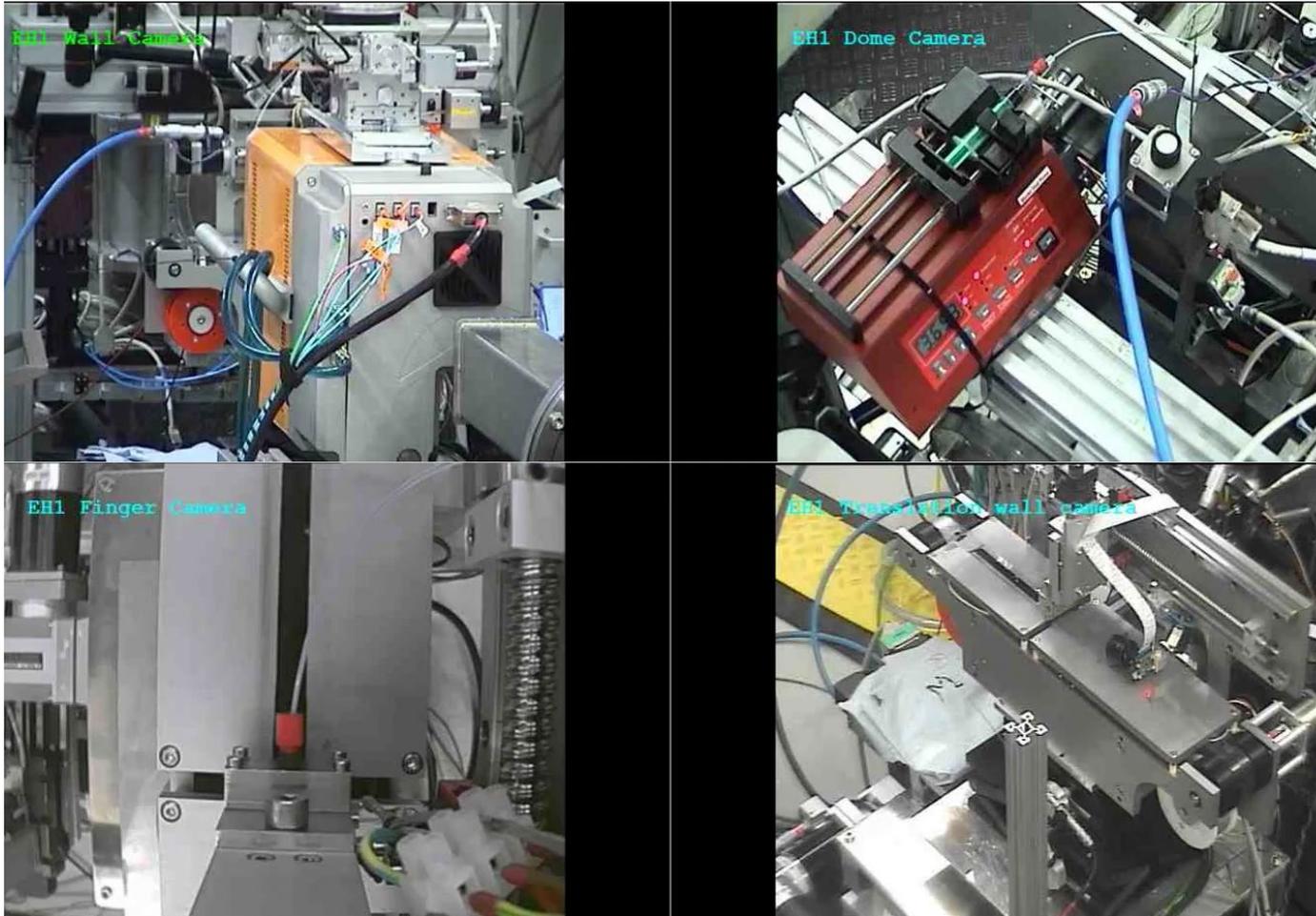
P03@PETRAIII DESY Hamburg



in situ X-ray scattering during hot-hot-hot roll-2-roll coating

4.
Validate structure

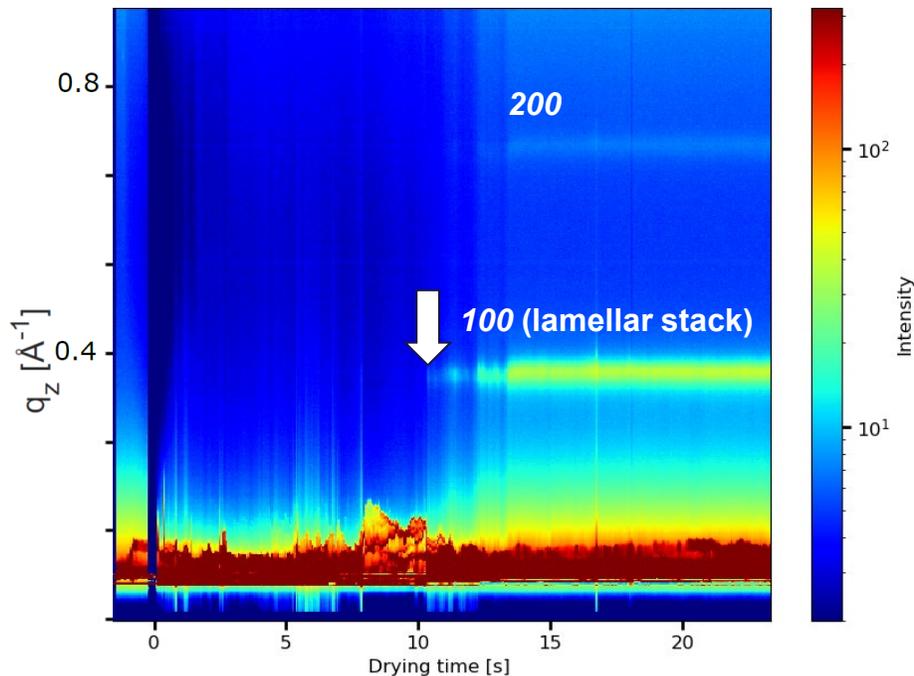
P03@PETRAIII DESY Hamburg



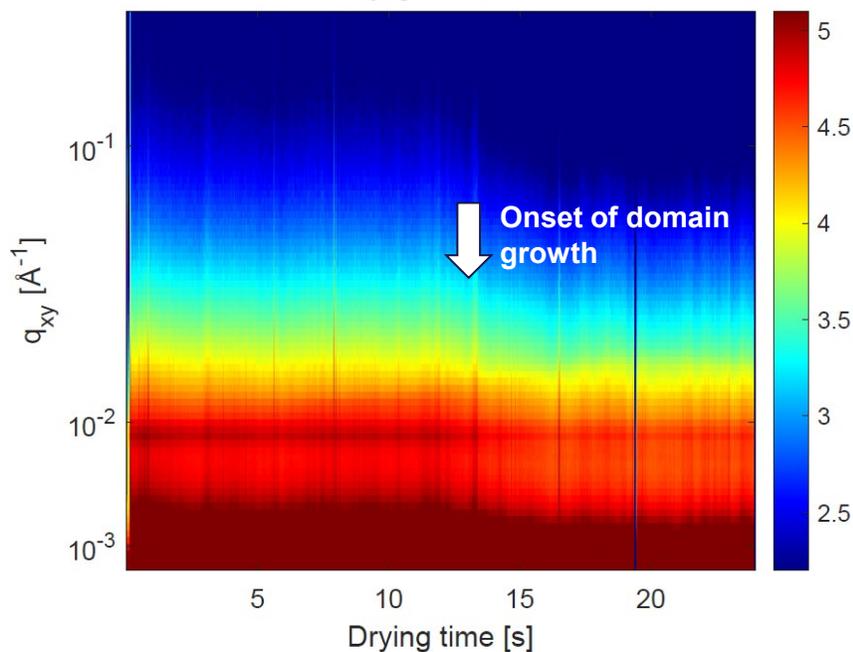
4.
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in situ X-ray scattering during hot-hot-hot roll-2-roll coating

GIWAXS

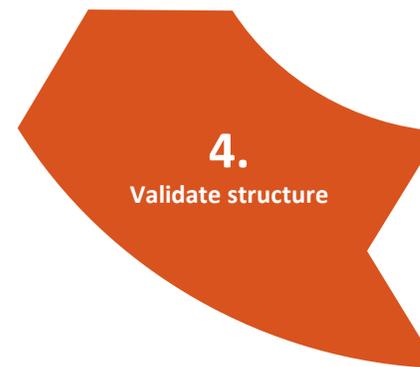


GISAXS

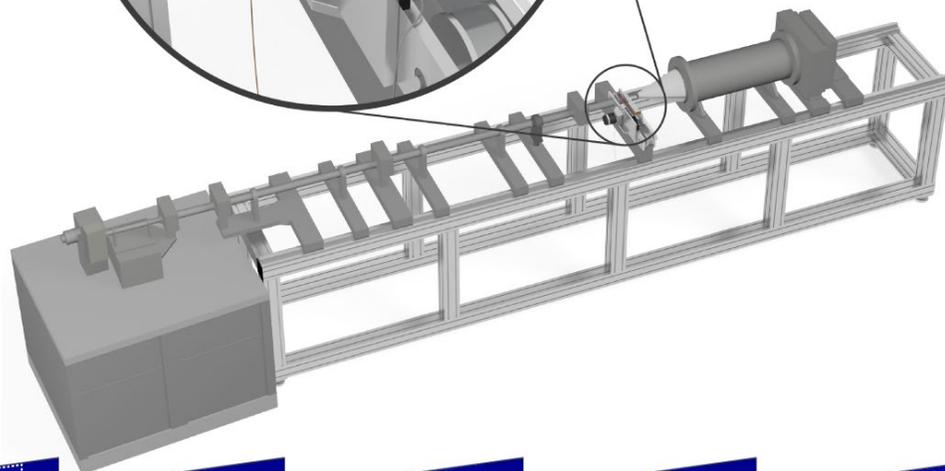
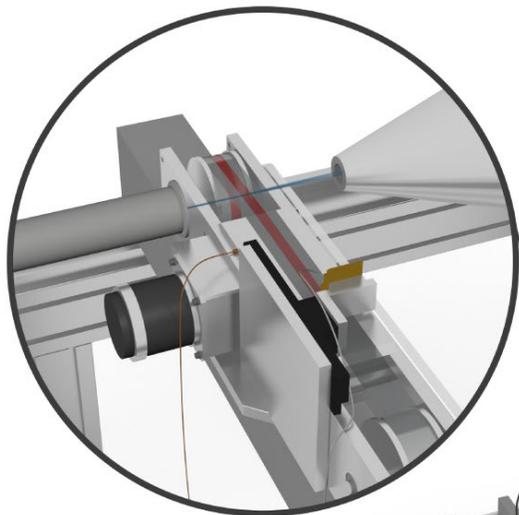


Correlation with MD meso-structure

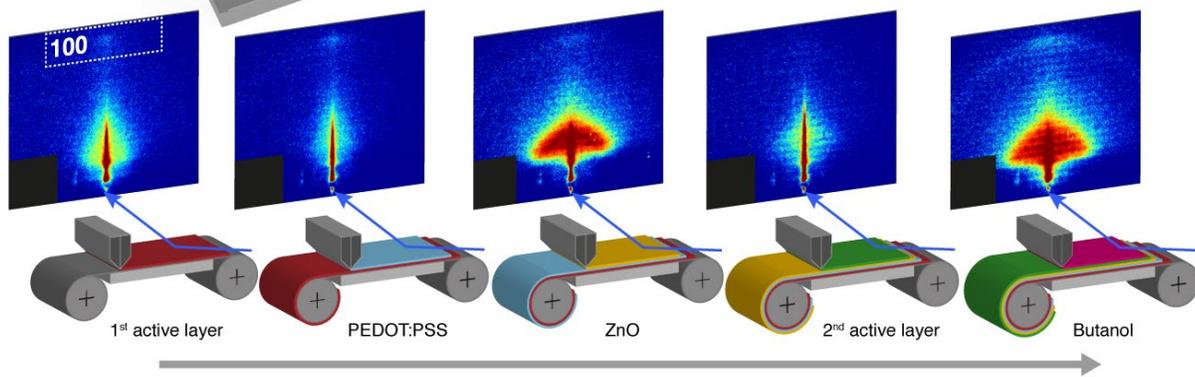
T_{process}	domain size, as-cast [nm]			domain size, annealed [nm]		
	298 K	333 K	363 K	298 K	333 K	363 K
OMA	5.88 ± 2.00	6.85 ± 1.69	6.79 ± 2.07	6.28 ± 1.13	7.69 ± 1.42	6.35 ± 1.37
CLBZ	7.96 ± 1.82	6.53 ± 1.12	6.69 ± 1.26	7.95 ± 0.83	7.25 ± 0.89	6.99 ± 1.27
OXYLE	7.39 ± 1.82	7.56 ± 1.83	7.26 ± 1.57	6.53 ± 0.84	7.31 ± 1.48	6.76 ± 1.43
DCLBZ	5.63 ± 1.13	9.71 ± 4.12	9.60 ± 2.50	6.80 ± 0.91	6.93 ± 1.91	9.38 ± 1.23
PCYM	5.93 ± 1.05	6.73 ± 2.15	5.69 ± 0.90	9.04 ± 3.07	7.15 ± 1.98	5.98 ± 0.97



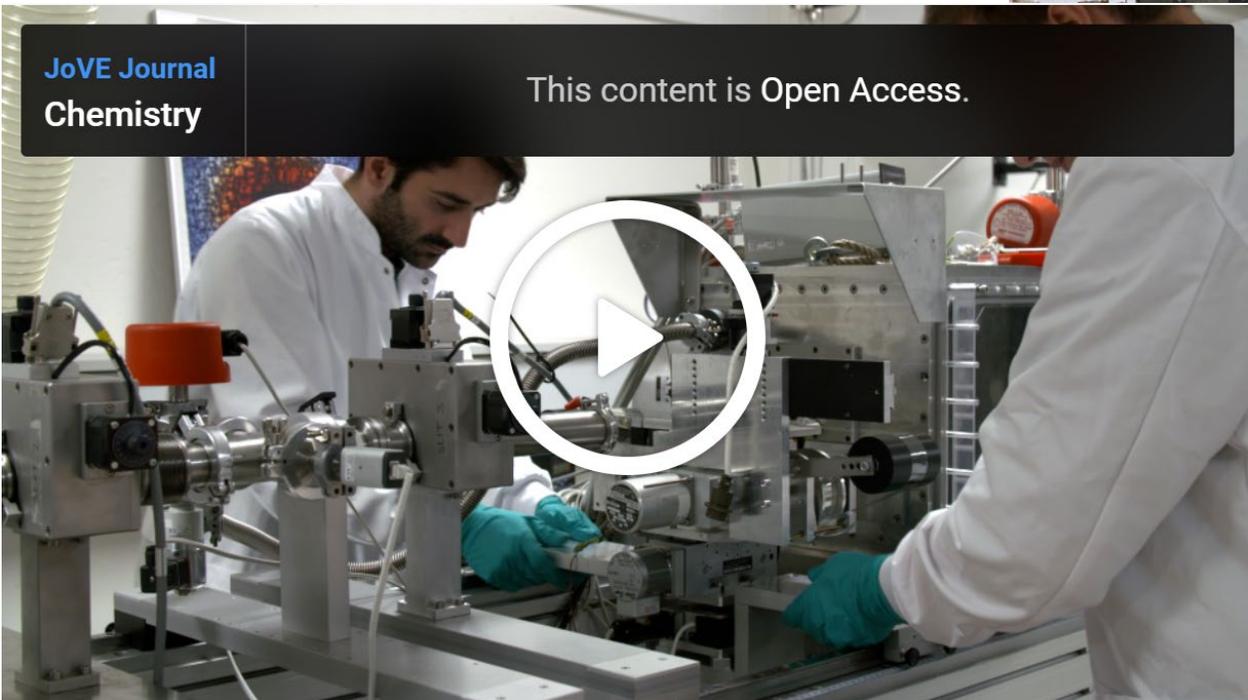
Unpublished results



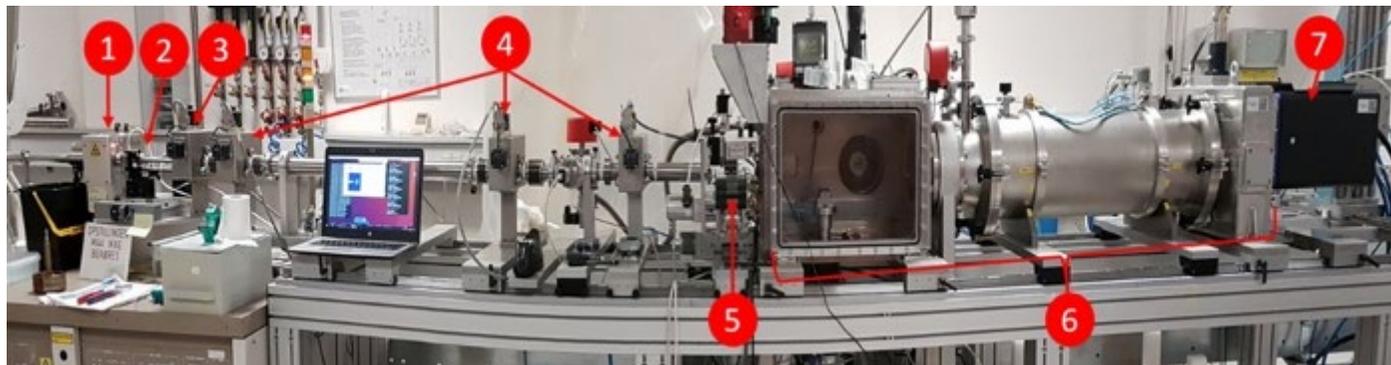
4.
Validate structure



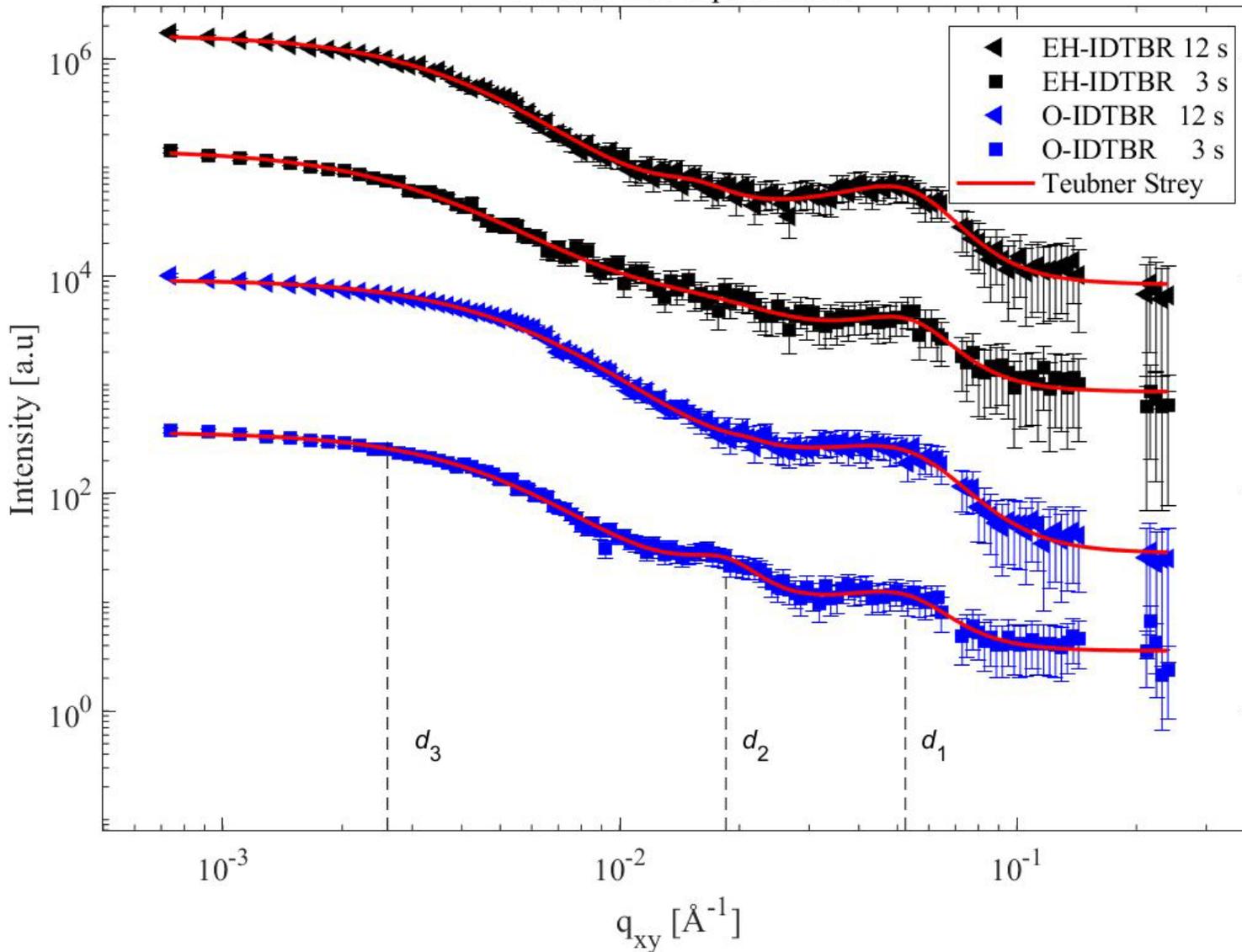
A I P Advances (2014), **4**, 087105
 Journal of Materials Chemistry A (2014), **2**, 18644–18654
 Advanced Energy Materials (2015), **5**, 1400736
 Energy Environ. Sci., (2017), **10**, 2411
 J. Visualized Experiments (2021), **169**, e61374



4.
Validate structure



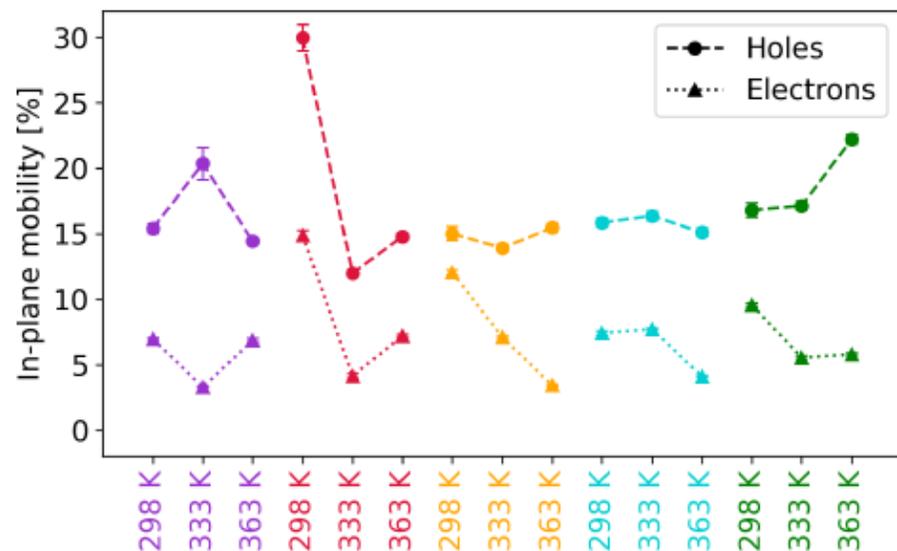
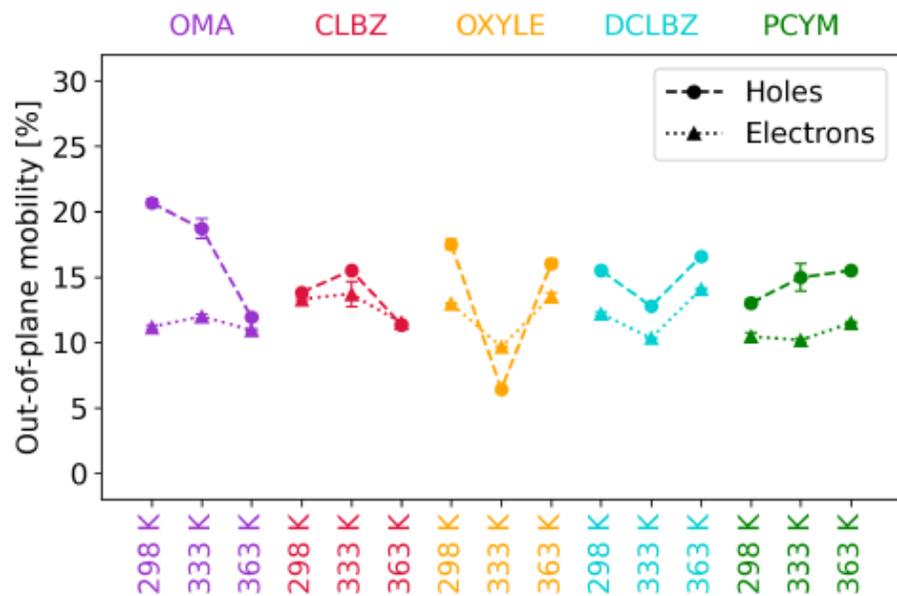
A I P Advances (2014), **4**, 087105
 Journal of Materials Chemistry A (2014), **2**, 18644–18654
 Advanced Energy Materials (2015), **5**, 1400736
 Energy Environ. Sci., (2017), **10**, 2411
 J. Visualized Experiments (2021), **169**, e61374



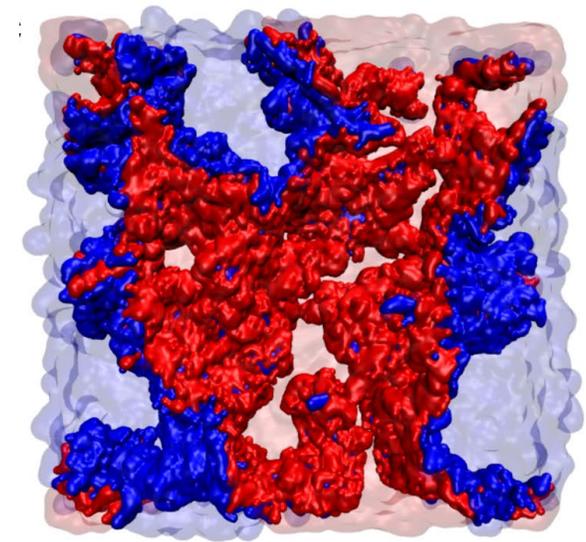
4.
Validate structure

Michael Korning Sørensen, Moises Espindola Rodriguez, Marcial Fernández Castro, Ashwin Nambi, Luise Theil Kuhn, Jens Wenzel Andreasen, In situ *Grazing Incidence Small Angle X-ray Scattering on Roll-To-Roll Coating of Organic Solar Cells with Laboratory X-ray Instrumentation*, *J. Visualized Experiments* (2021), **169**, e61374

P3HT:O-IDTBR



5.
Predict performance



Normalized time-of-flight charge carrier mobilities from kMC simulations in the out-of-plane direction (z-direction; left column) and in the in-plane direction (average of x- and y-directions; right column) for annealed P3HT:O-IDTBR systems

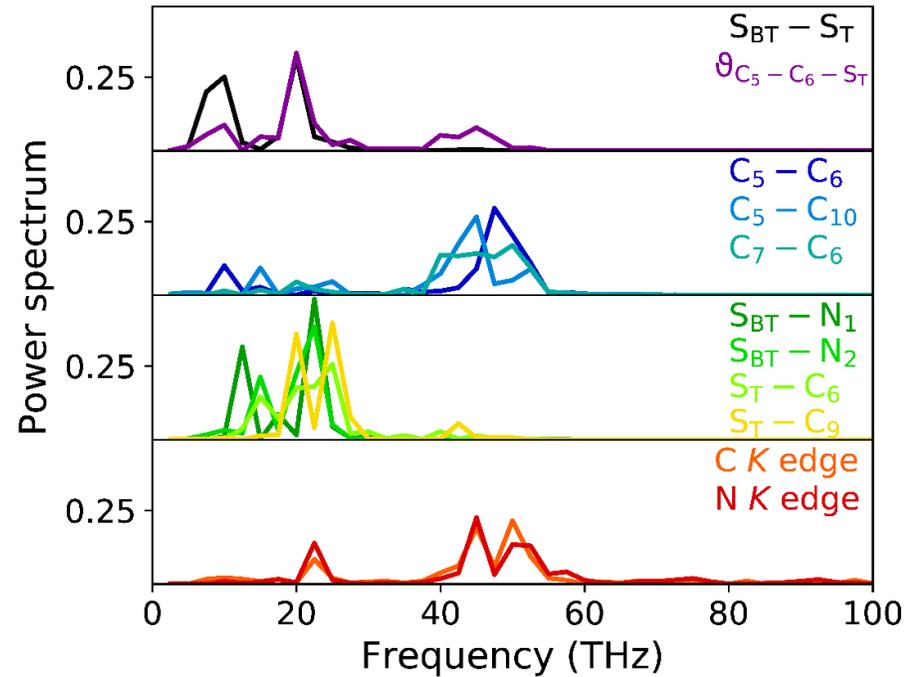
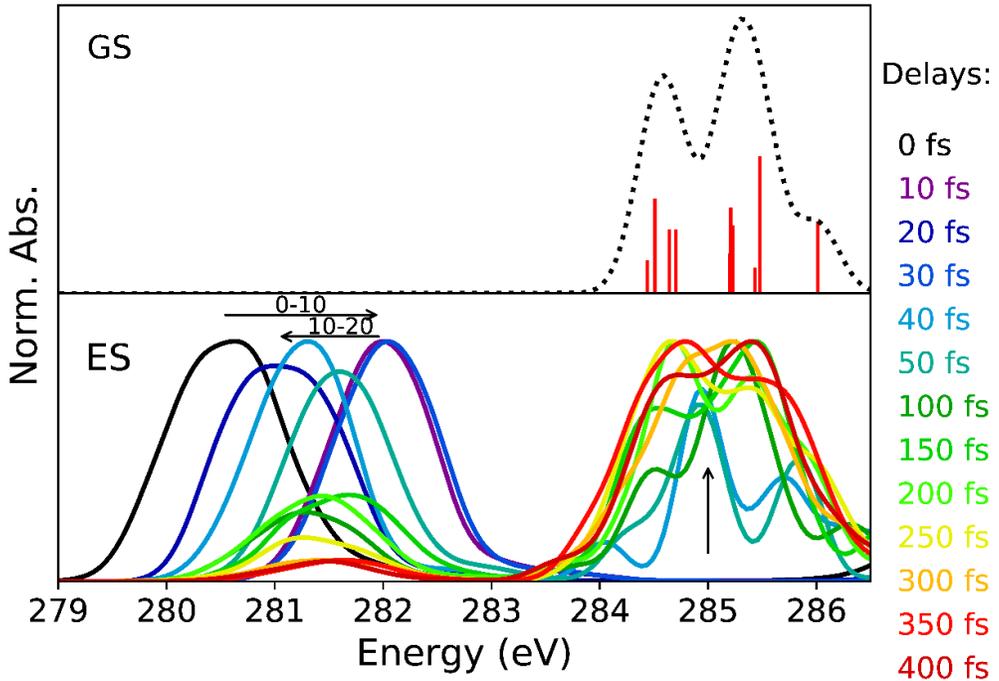
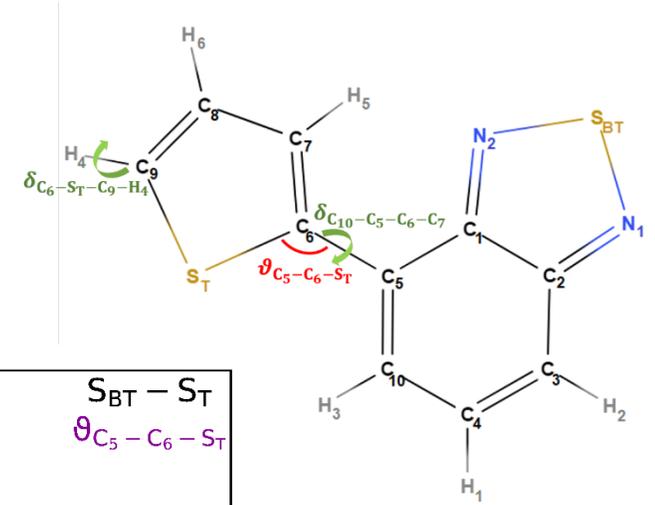
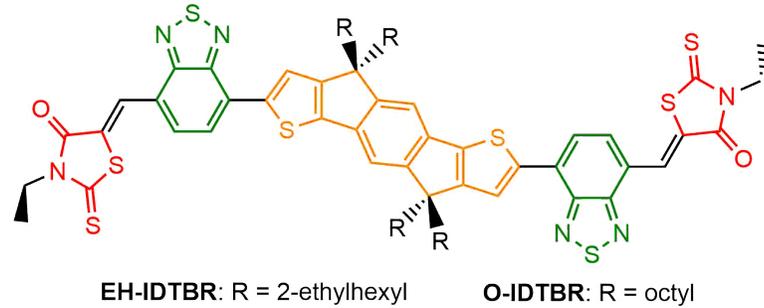
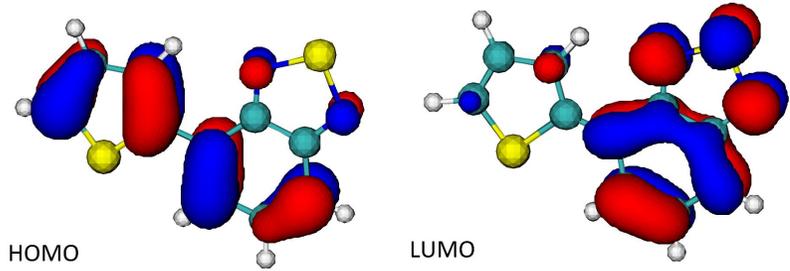
6.
 Validate performance

Average device properties (six cells or more) of 1 cm^2 , flexible P3HT:O-IDTBR organic solar cells with slot-die coated active layers processed from different solvents and at different temperatures.

	$T_{\text{process.}}$	OMA	CLBZ	OXYLE	DCLBZ	PCYM*
PCE [%]	333 K	3.19 ± 0.17	1.84 ± 0.07	2.63 ± 0.18	2.14 ± 0.21	2.79 ± 0.08
	363 K	1.39 ± 0.18	1.46 ± 0.06	1.52 ± 0.21	1.70 ± 0.18	1.97 ± 0.43
FF [%]	333 K	59.2 ± 1.2	38.6 ± 1.3	49.7 ± 2.5	44.6 ± 4.2	56.9 ± 1.8
	363 K	36.8 ± 2.1	33.2 ± 1.2	36.8 ± 2.2	40.1 ± 1.9	43.1 ± 9.2
$J_{\text{sc}} \left[\frac{\text{mA}}{\text{cm}^2} \right]$	333 K	7.54 ± 0.35	6.66 ± 0.12	7.35 ± 0.48	6.68 ± 0.21	6.90 ± 0.00
	363 K	5.28 ± 0.40	6.06 ± 0.27	5.92 ± 0.35	5.76 ± 0.44	6.38 ± 0.32
$V_{\text{oc}} \text{ [V]}$	333 K	0.72 ± 0.00	0.71 ± 0.01	0.72 ± 0.00	0.72 ± 0.01	0.72 ± 0.00
	363 K	0.71 ± 0.01	0.72 ± 0.01	0.73 ± 0.01	0.73 ± 0.01	0.72 ± 0.01

*values for PCYM at 333 K are averages of only three cells

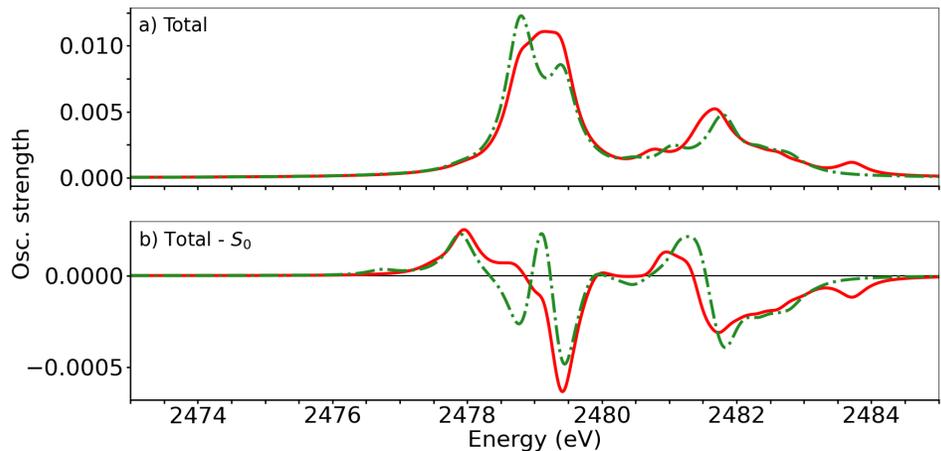
Back to fundamentals: Simulation of Time-Resolved X-ray Absorption Spectroscopy of Ultrafast Dynamics in BT1T



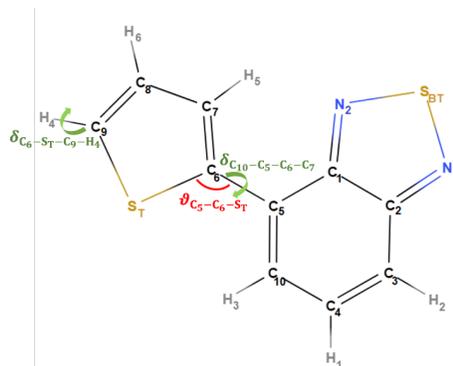
Simulation of time-resolved X-ray absorption spectroscopy of ultrafast dynamics in particle-hole-excited 4-(2-thienyl)-2,1,3-benzothiadiazole
 Khadijeh Khalili, (...) Jens Wenzel Andreasen* & Robin Santra
 Structural Dynamics **7**, 044101 (2020)

DTU First free-electron X-ray laser experiments on an organic donor-acceptor dyad

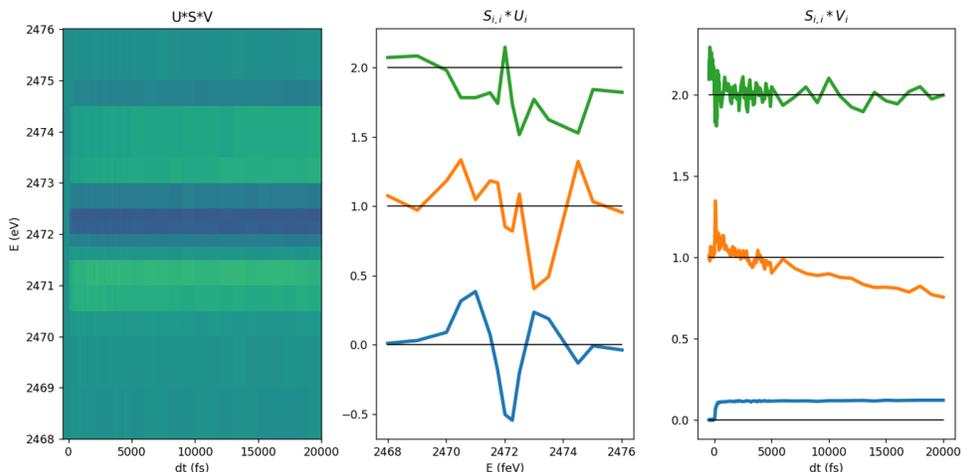
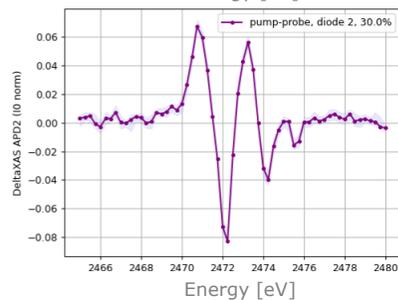
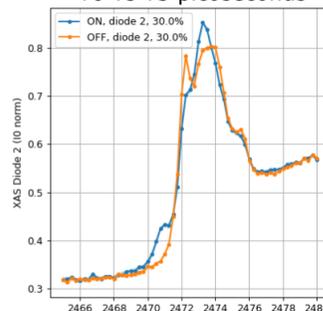
— fc-CVS-EOM-CCSD — BHHLYP, $\Delta = 31.46$ eV



— fc-CVS-EOM-CCSD — BHHLYP, $\Delta = 31.46$ eV



T0 vs T5 picoseconds





Wagner, J., Berger, C.G., Du, X. *et al.* The evolution of Materials Acceleration Platforms: toward the laboratory of the future with AMANDA. *J Mater Sci* **56**, 16422–16446 (2021)



Outlook:

The roll-2-roll platform is the ideal high-throughput scalable testing platform for model-supported, AI-guided exploration of materials and processing for scalable, stable organic solar cells based on non-fullerene acceptors

DTU Acknowledgements



Solar Energy Enabled for the World by High resolution Imaging
Funded by:



European Research Council
Established by the European Commission

