武漢大學 高等研究院
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Modification of Metastable Phase in Organic Solar Cells (Degree of Polymerization)

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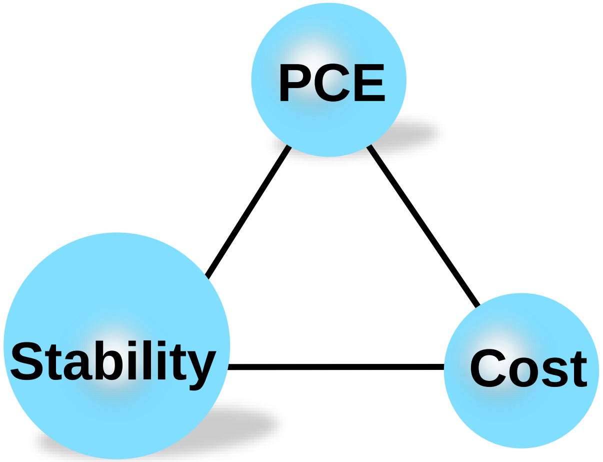
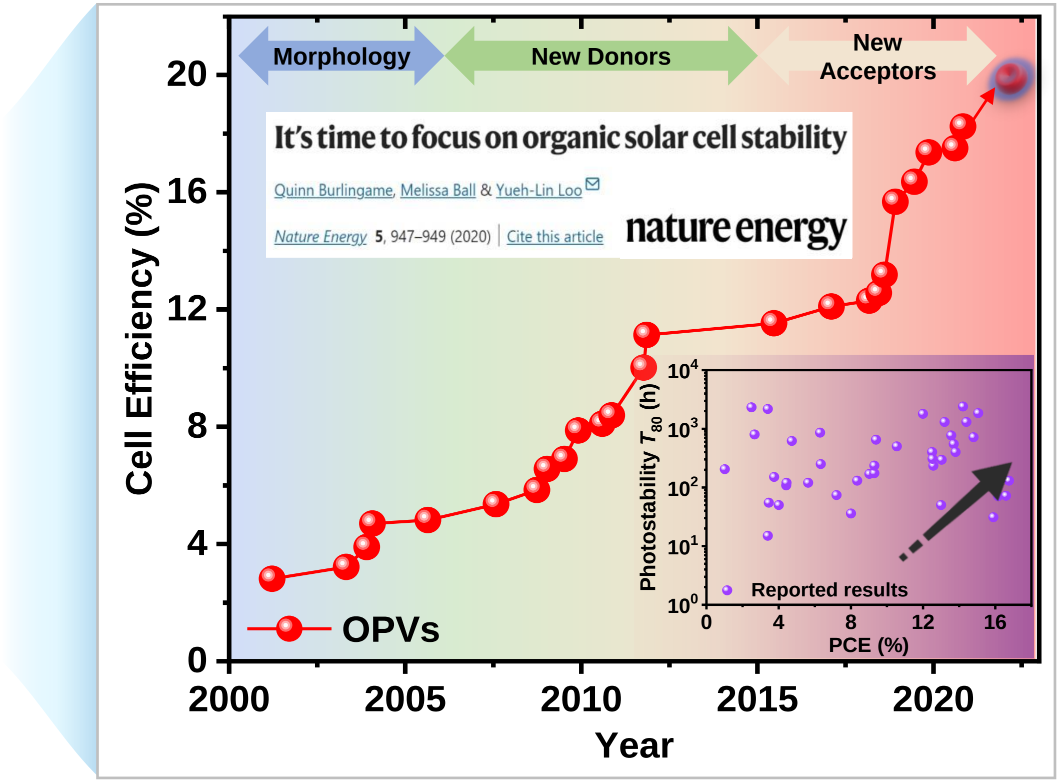
Research status

Dramatic advances in PCEs achieved in these five years



Golden triangle of solar cells

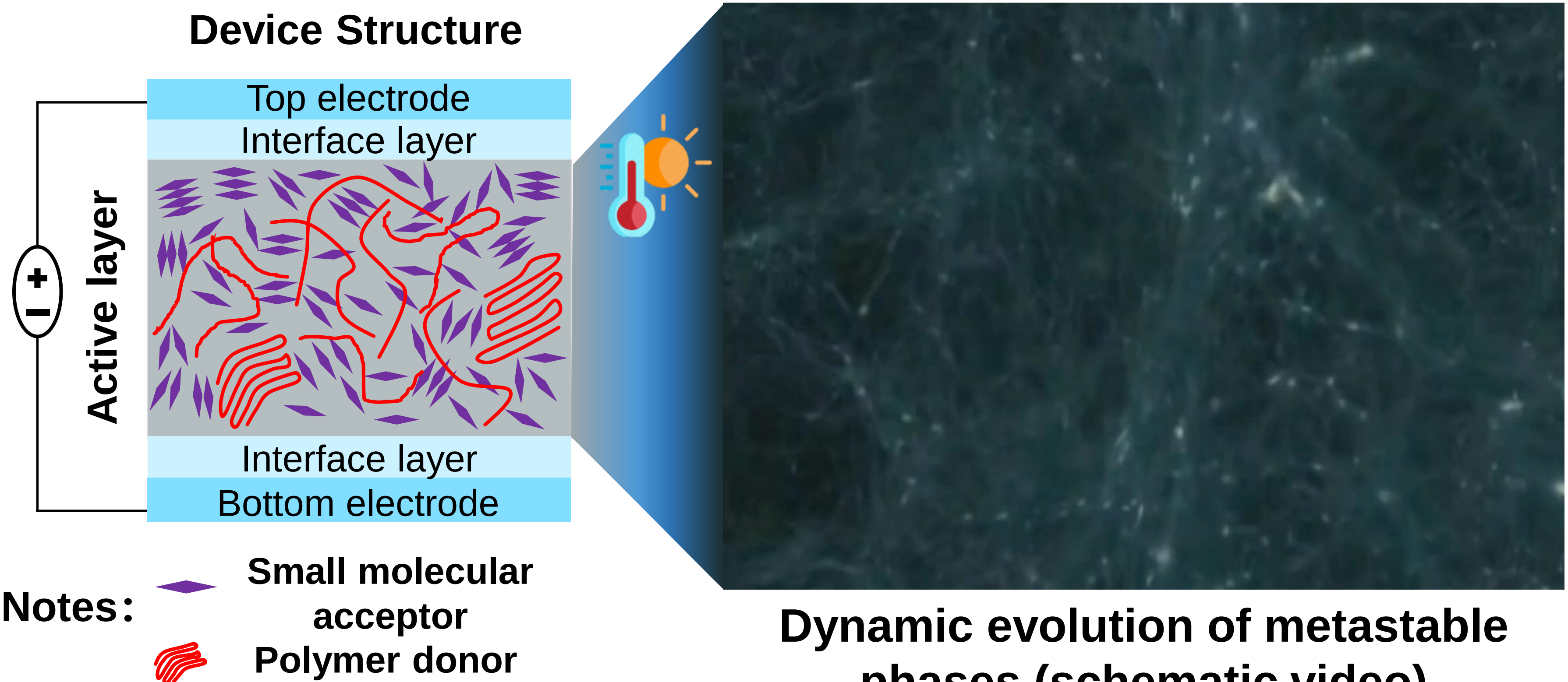


A big lifetime issue:

Current active layer systems can not meet the requirements for long-term operation

Key scientific issues

Key point: **How to precisely regulate the metastable phase and suppress the phase evolution?**

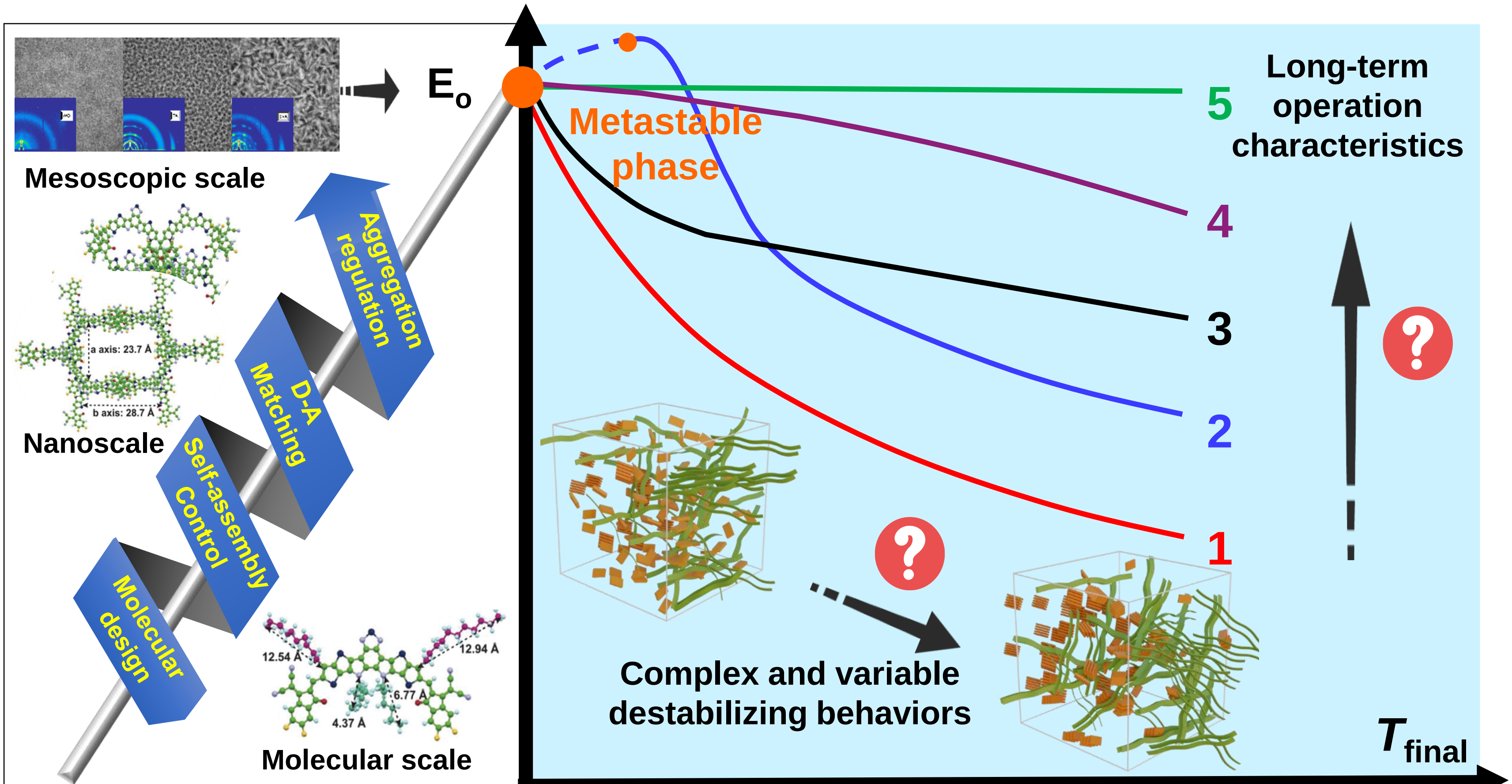


Dynamic evolution of metastable phases (schematic video)

Metastable phase evolution mechanisms

Aggregation regulation (material properties)

Metastable phase modification (mixed-phase domain)

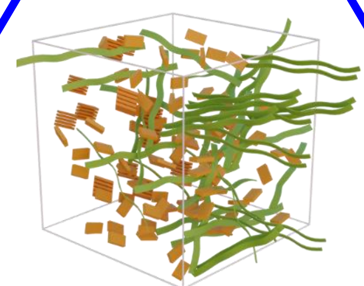


Research idea: Understanding the destabilizing behaviors of ALs; Guiding molecular design and morphology control

Research content

Degradation behaviors

The instability mechanism of high-efficiency metastable active layer



Acceptor molecular design to modify the A/A and D/A interactions in blends

Process control

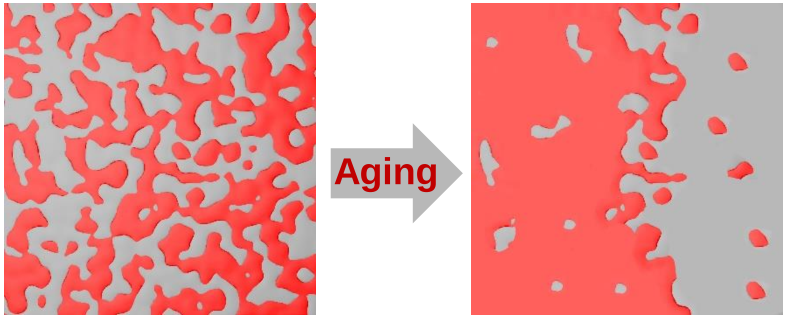
Materials design

Phase reconstruction to improve the practicability of OPV materials

Morphological instability of mixed phase domain

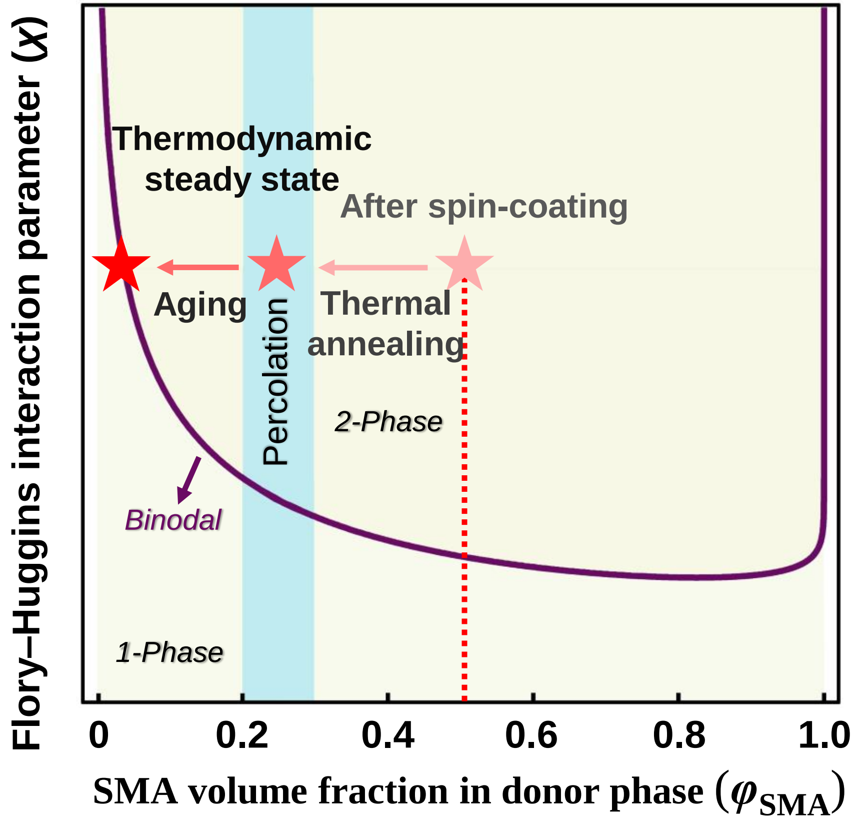
Intrinsic factors: molecular structure and intermolecular interactions

Morphology evolution under operating conditions



Bi-continue interpenetrating network structure

- ✓ **Over-purified phase domain**
- ✓ **Large phase separation size**



$$D(\mathrm{T}) \propto \frac{1}{\mathrm{T_g}}$$

D(T): Molecular diffusion coefficient

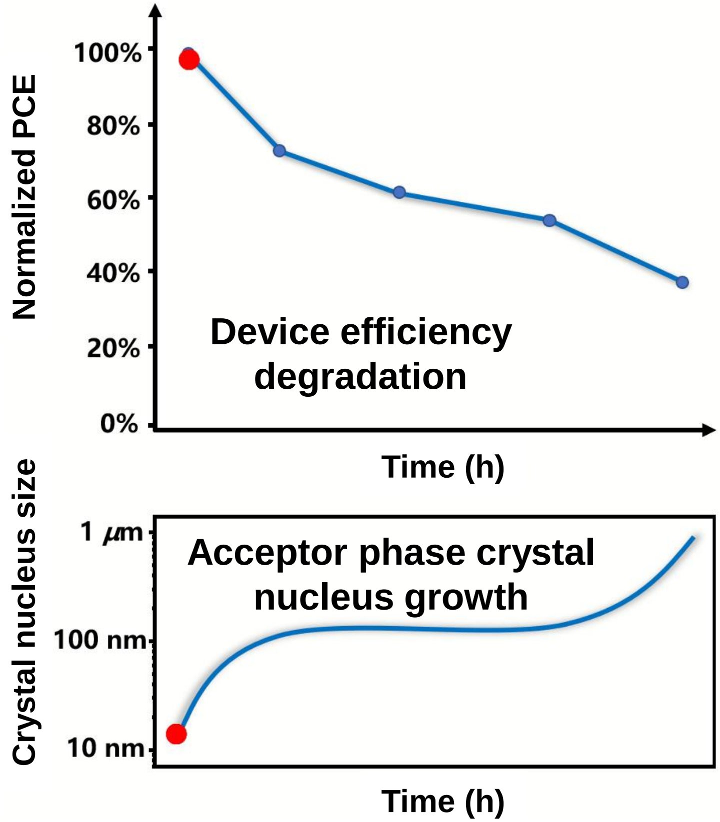
T_g: Phase transition temperature

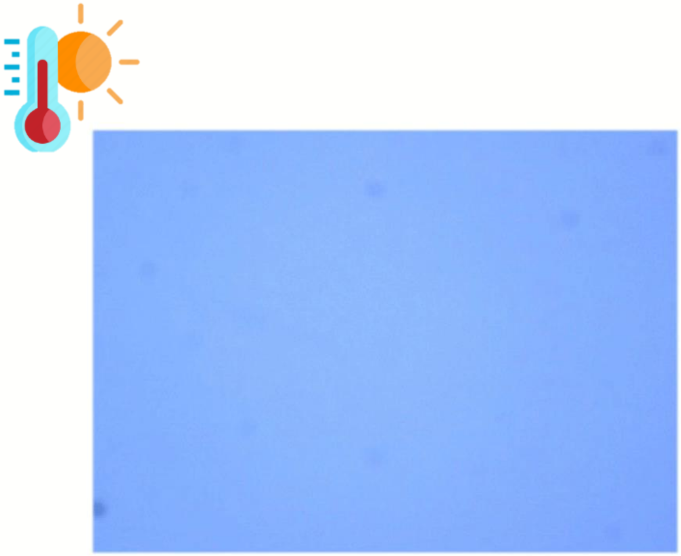
Relative miscibility (D/A)

$$\frac{\chi_{1,2}}{\chi_{Spinodal}} = \frac{2}{RT}\frac{(\delta_{T1}-\delta_{T2})^2}{\left(\frac{\rho_1}{M_1\phi_1}+\frac{\rho_2}{M_2(1-\phi_1)}\right)}$$

Destabilization mechanism of PD:SMA

1. Amorphous mixed phase demixing → **2. Small isolated domain formation** → **3. Donor/acceptor crystal phase separation**



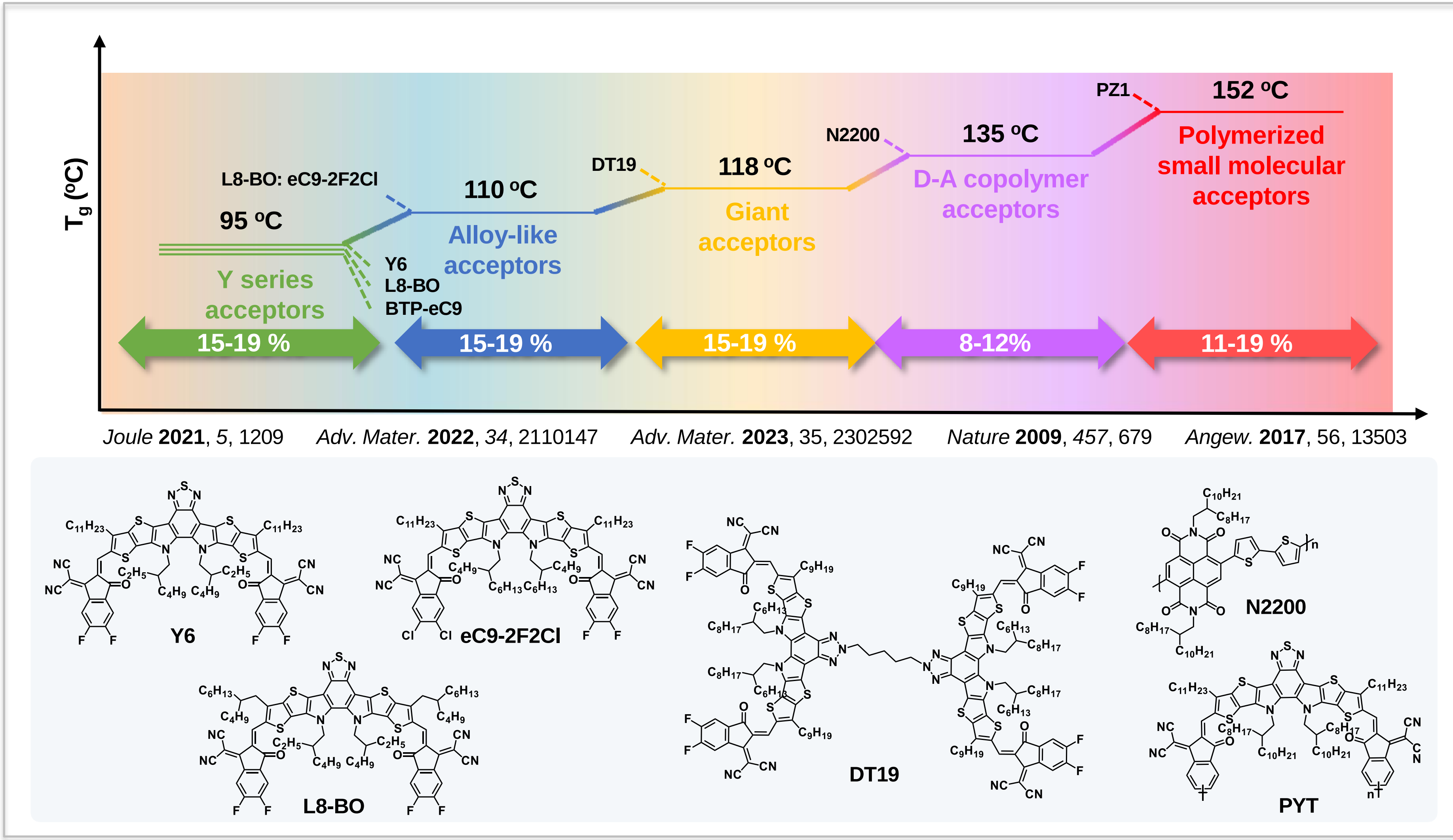


Metastable phase evolution
Recorded by optical microscope

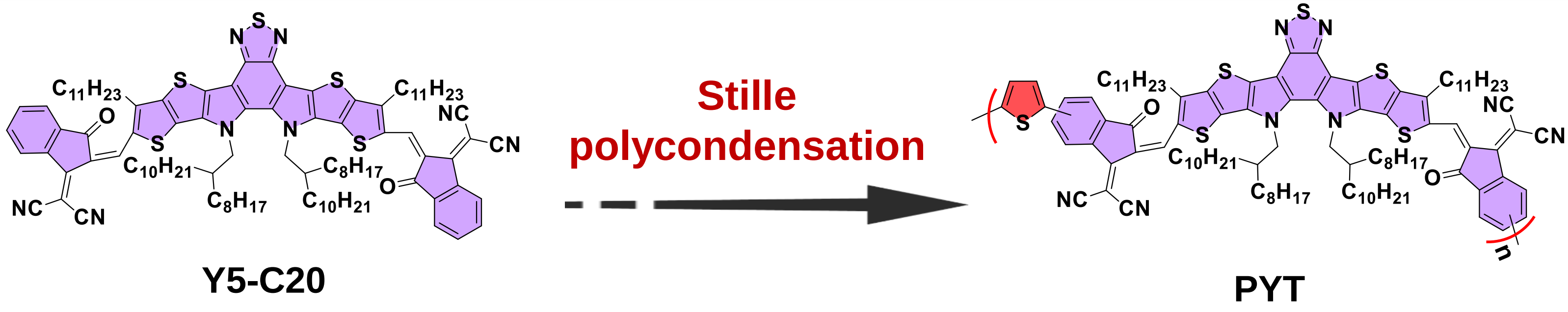
J. Min* *et. al. Adv. Mater.*, **2023**, 35, 2302592.

Explore the evolution mechanisms of blend phase

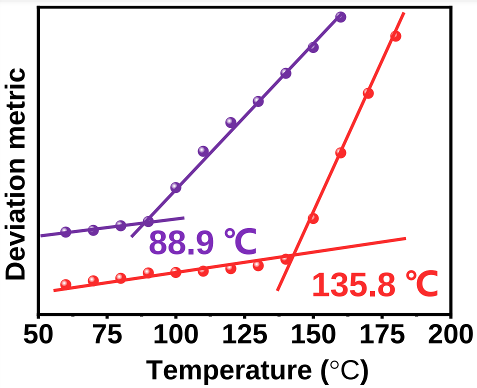
The analysis focused on the T_g of various acceptor materials



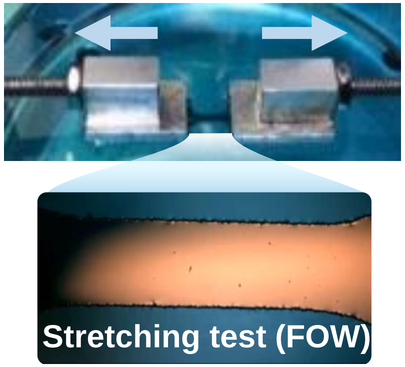
Design and synthesis of PSMAs



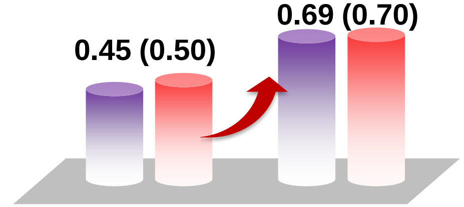
First group to introduce Y-series acceptor into polymer acceptors



T_g improved 70%



Ultimate tensile strain (ε) enhanced to 3-10 times



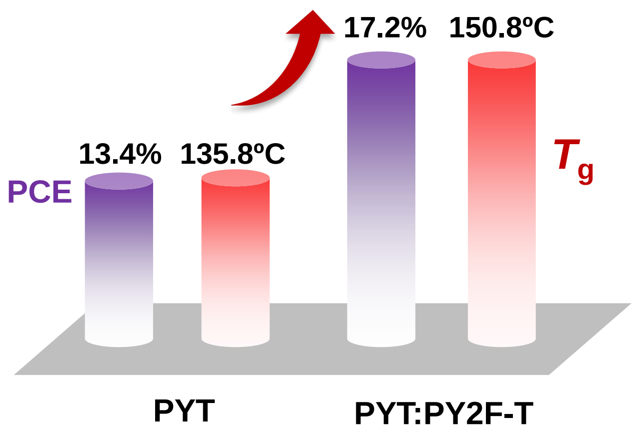
Initial PCE 9.4% → 13.4%

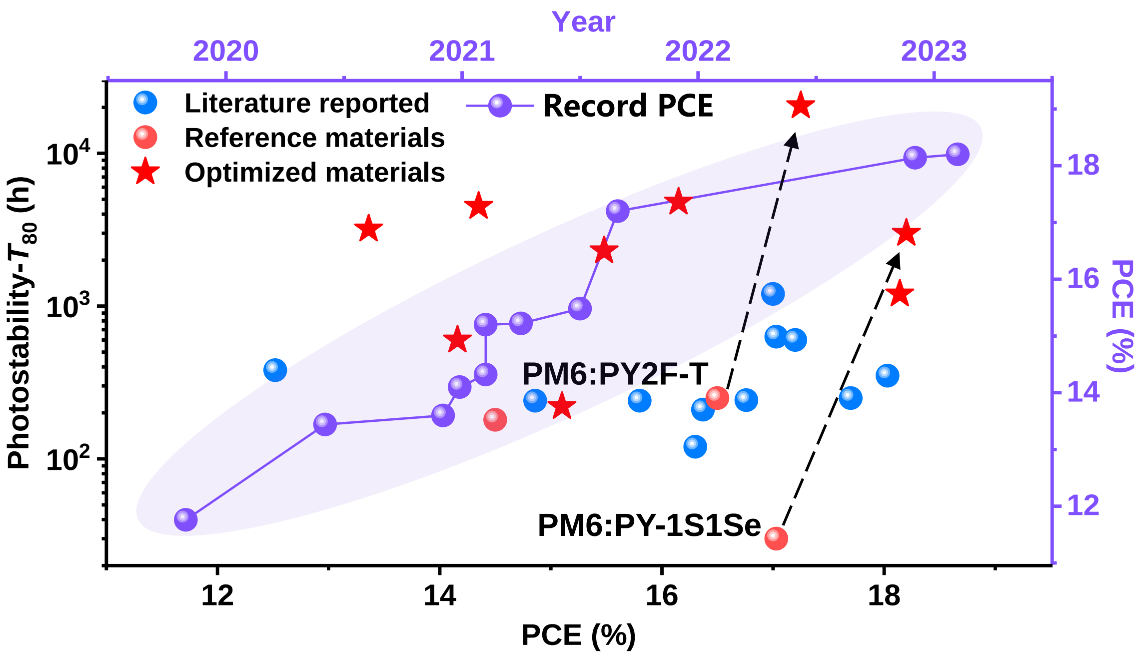
High M_w→Viscoelastic effect
enhancing T_g values, mechanical and operational stability

*J. Min** *et. al. Joule* **2020**, *4*, 1086; *Sci. China Chem.*, **2020**, *63*, 1449.

Efficient and stable all-polymer systems

Multiple strategies: increasing the T_g of A materials
optimizing the metastable morphology



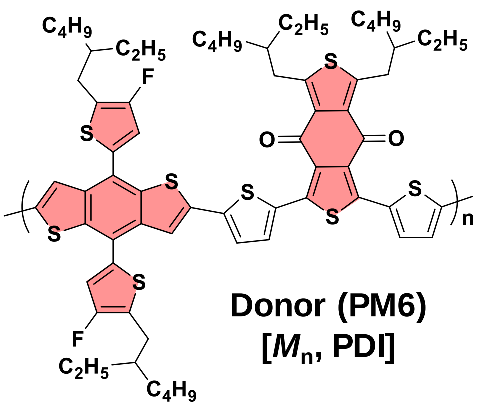


PCE (11.7%→19.0%) and operational stability (T_{80}=35,000 hours)

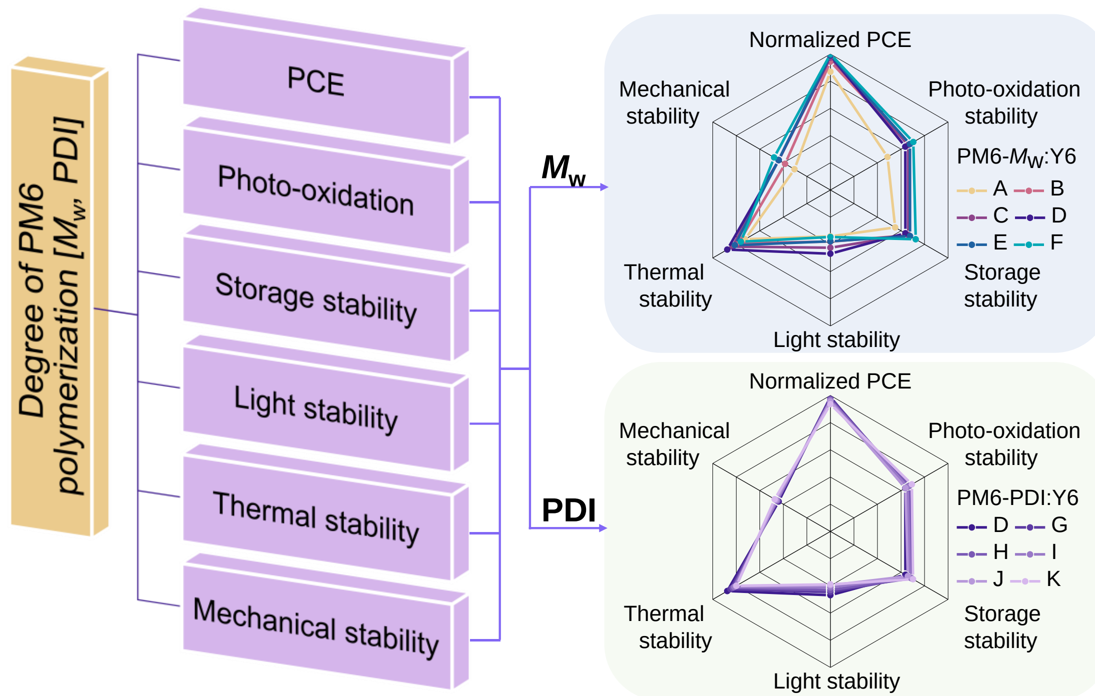
*J. Min** *et. al. Chem* **2023**, *9*, 1702; *Joule* **2021**, *5*, 1548; *EES* **2024**, *Under Review*.

Degree of polymerization → Intermolecular interactions

DP control: modify D/D and D/A interactions control active layer morphology



Donor (PM6) [M_n, PDI]

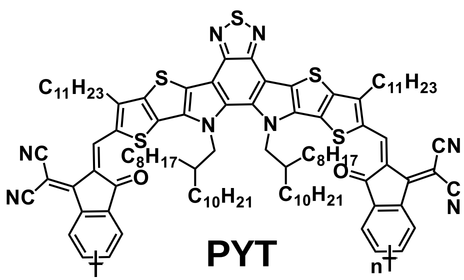


Batch	A	B	C	D	E	F	G	H	I	J	K
M_n [kDa]	28.1	44.1	68.7	73.8	80.8	97.6	72.3	73.9	71.6	75.5	74.0
PDI	2.68	2.63	2.29	2.16	2.12	2.07	2.36	2.59	2.74	3.05	3.60

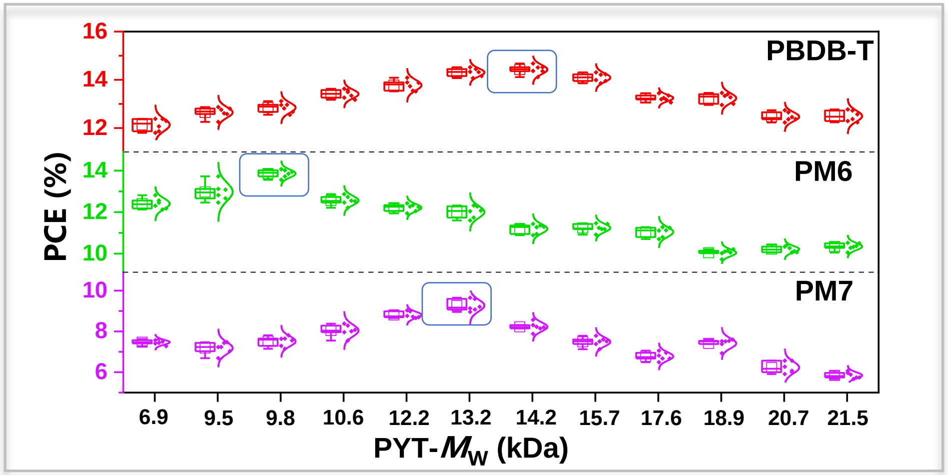
J. Min et. al. Adv. Energy Mater.*, **2020**, 10, 2002709.

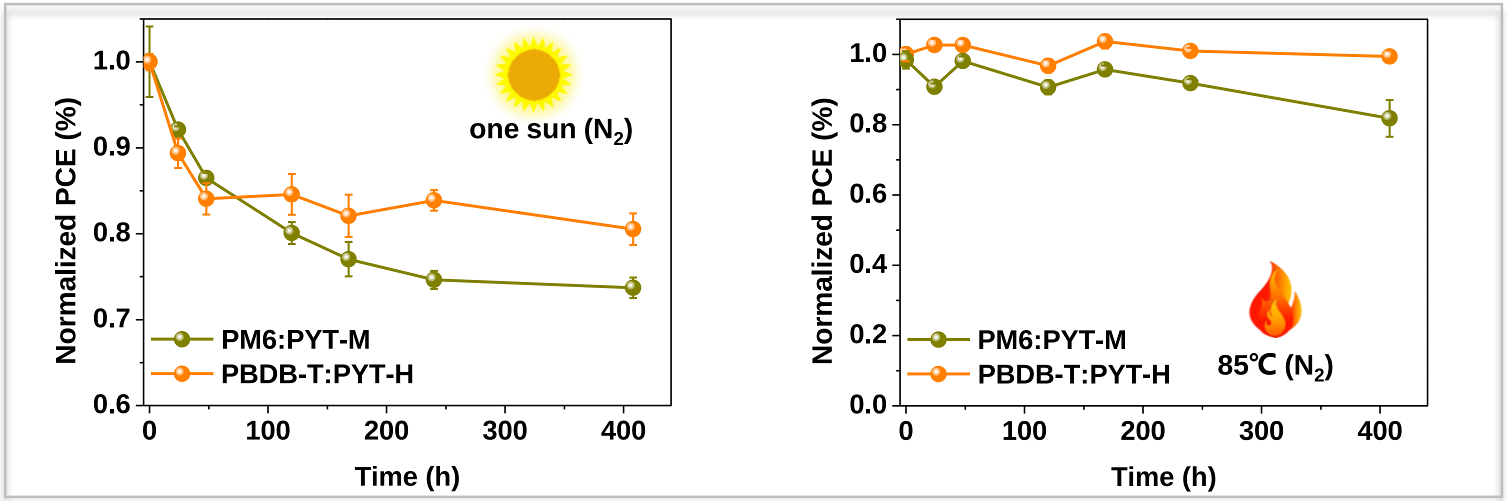
DPs of PYT

M_w: modify D/A miscibility, **determine device efficiency and stability**



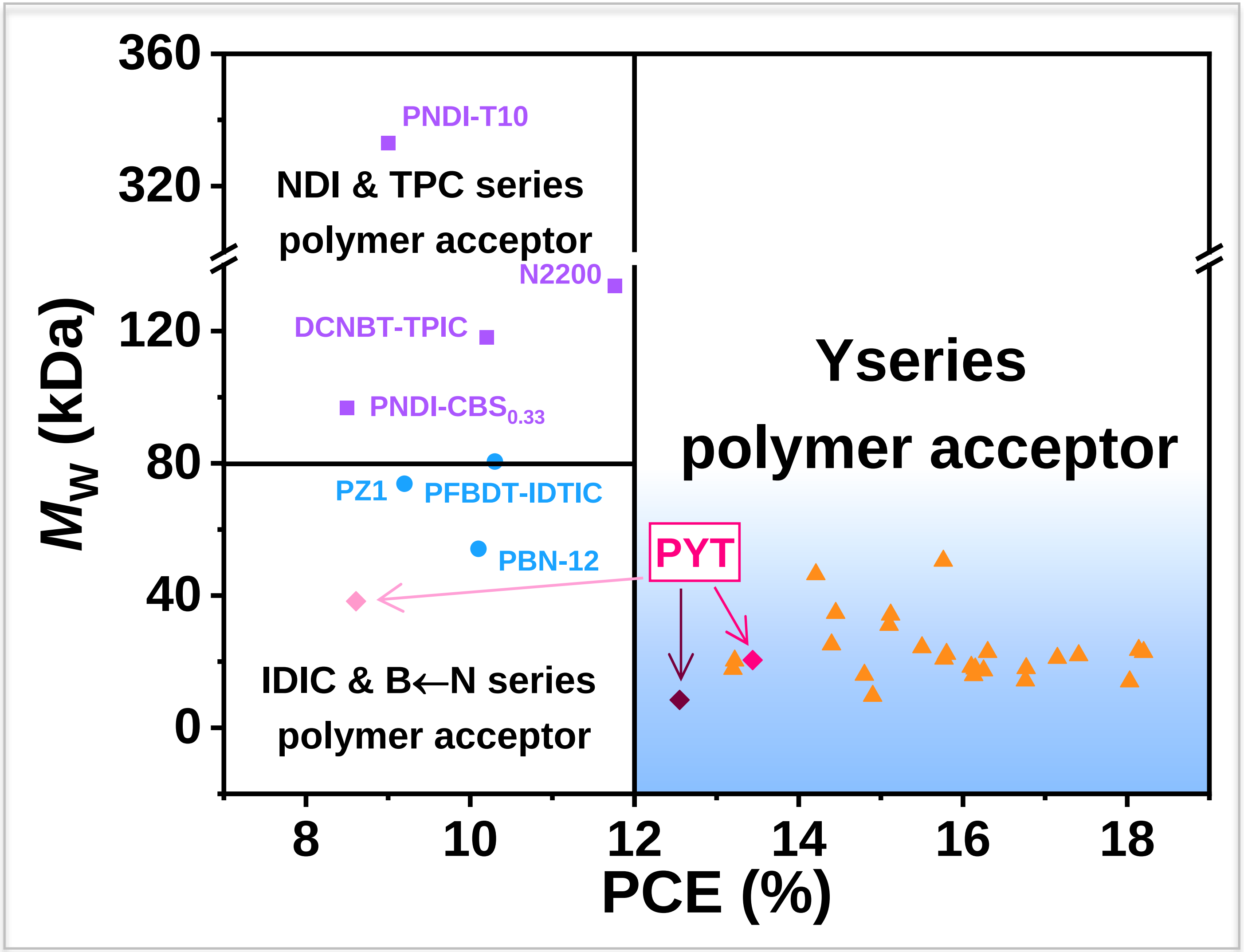
Influence of M_ws on device performance





*J. Min** *et. al. Joule*, **2020**, 4, 1070; *J. Mater. Chem. C.*, **2022**, *10*, 1850.

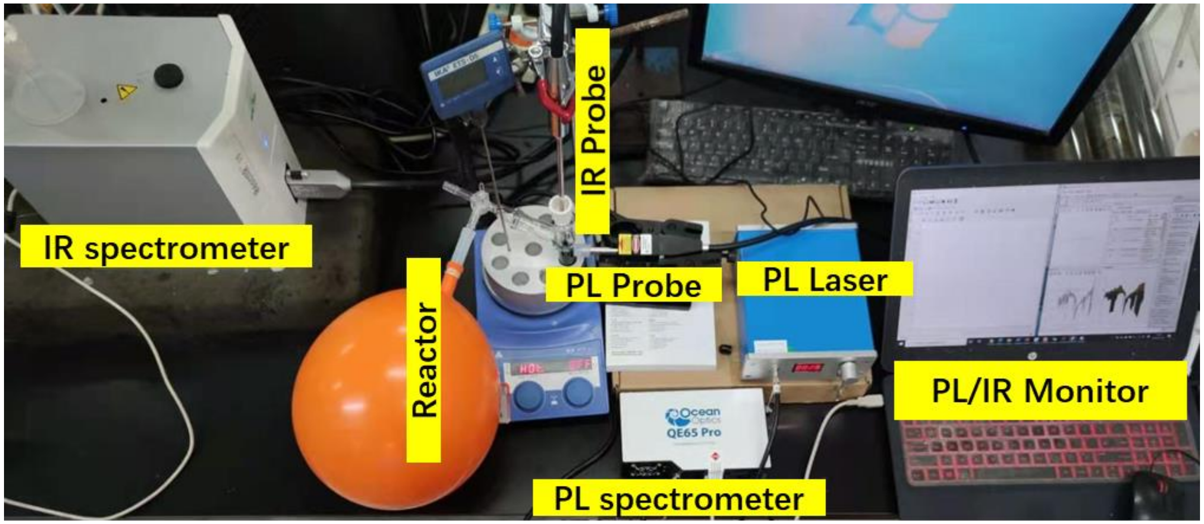
Precision synthesis (Fronting phase regulation)



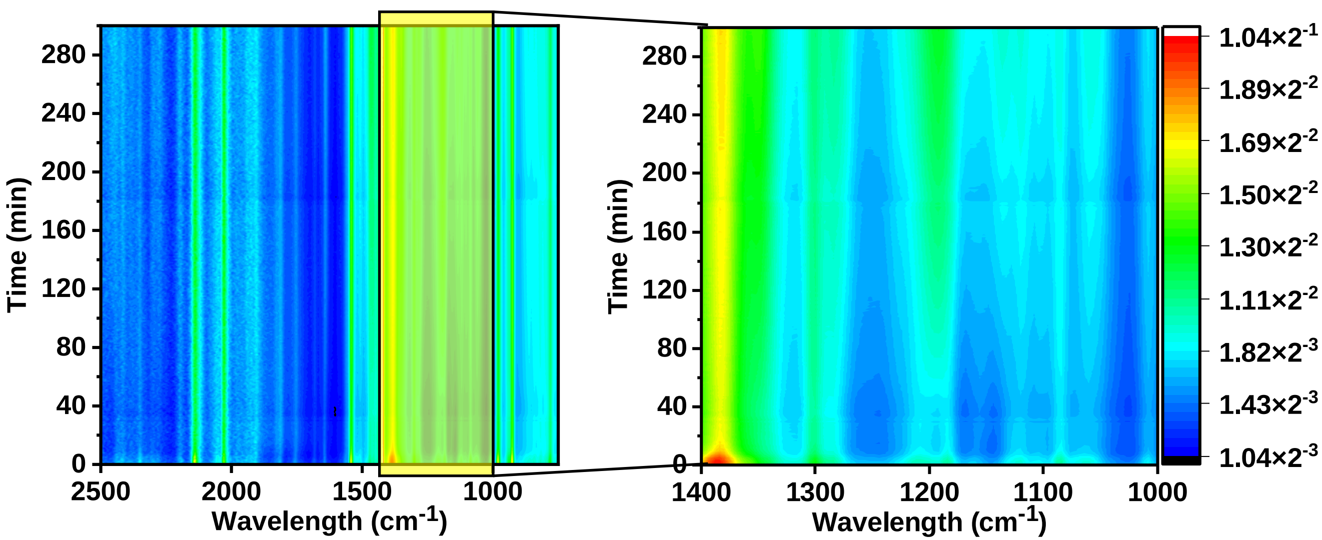
*J. Min** *et. al. Joule* **2020**, *4*, 1086; *Sci. China Chem.*, **2020**, *63*, 1449.

Development of a real-time polymerization detection system

Methods: Combined *in-situ* FTIR and PL spectroscopy (**process control**)



***In-situ* FTIR spectrum**



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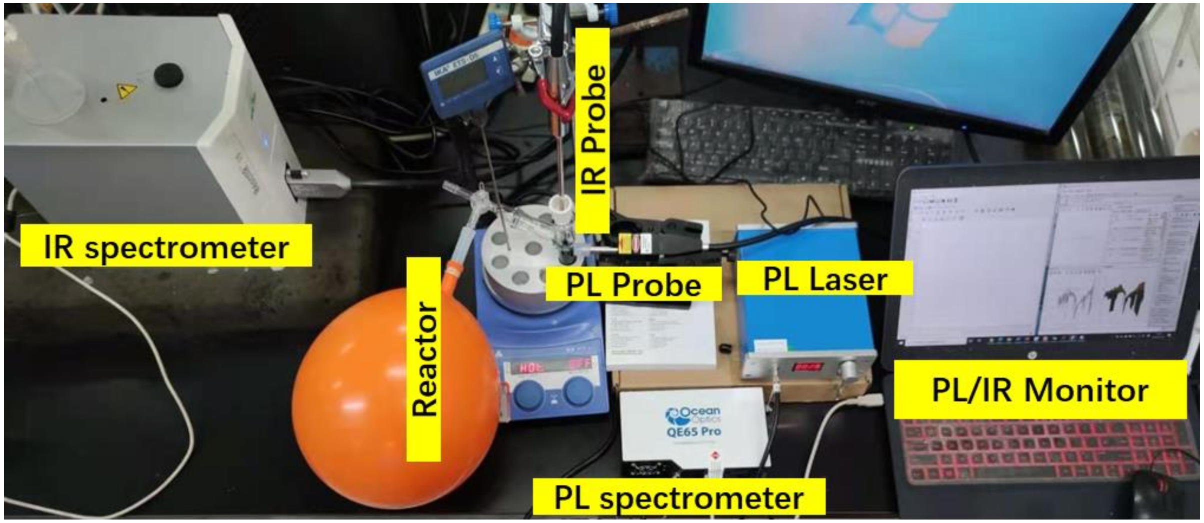
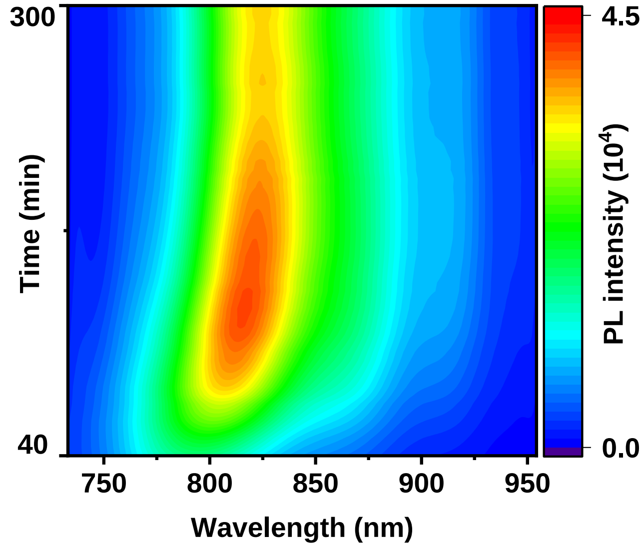
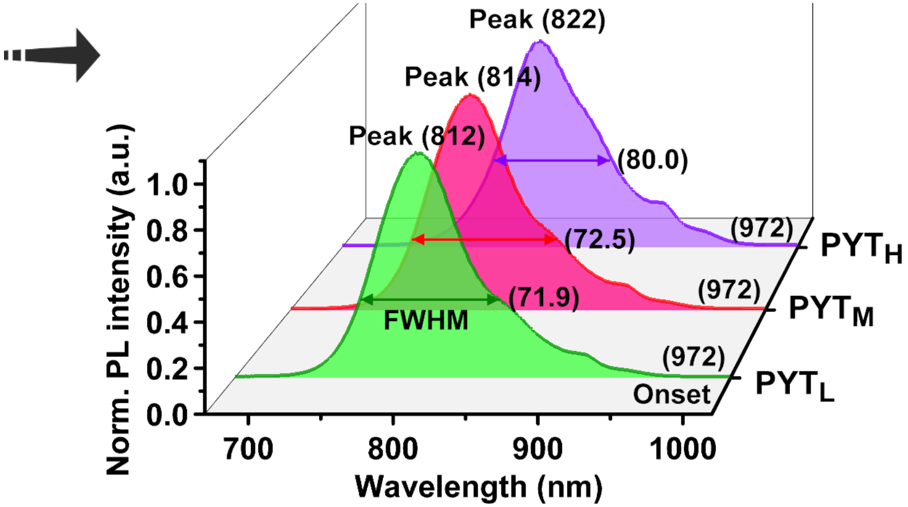


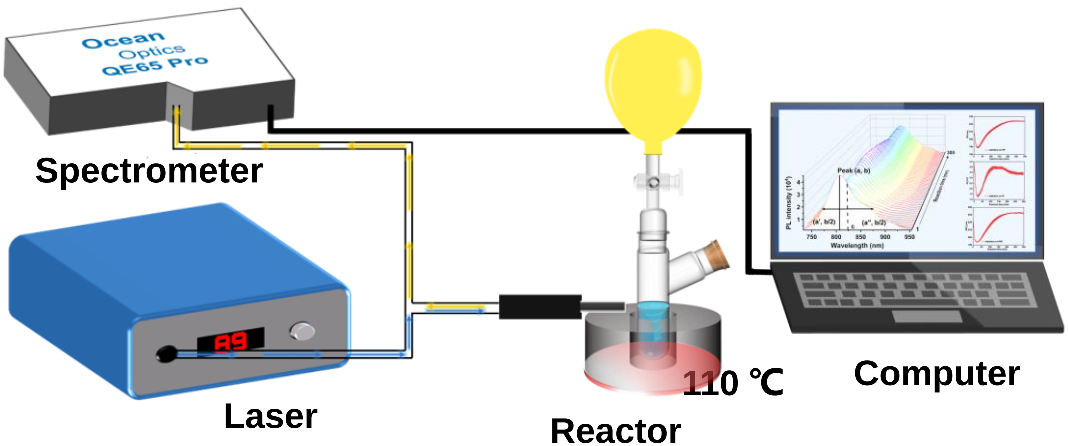
***In-situ* PL spectrum**

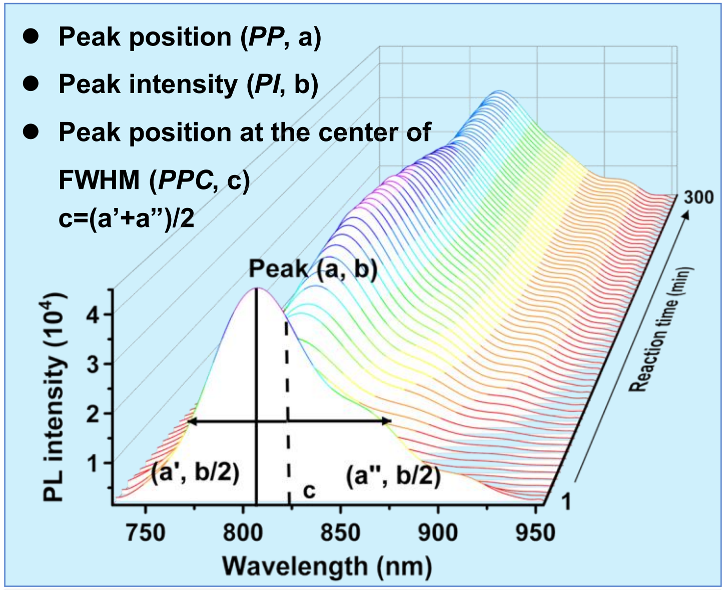


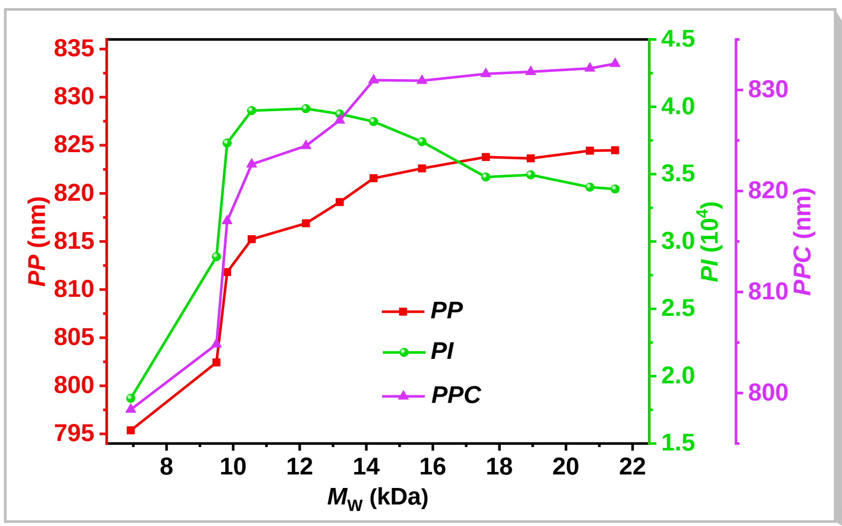


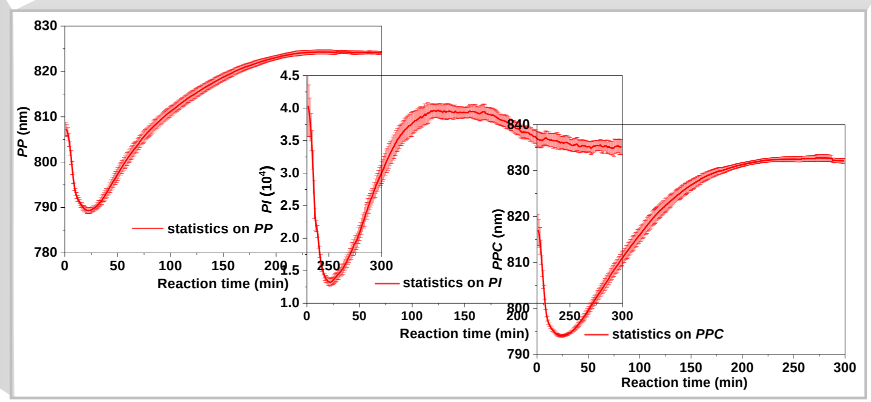
Development of a real-time polymerization detection system

Method: Automatic polymerization monitoring technology









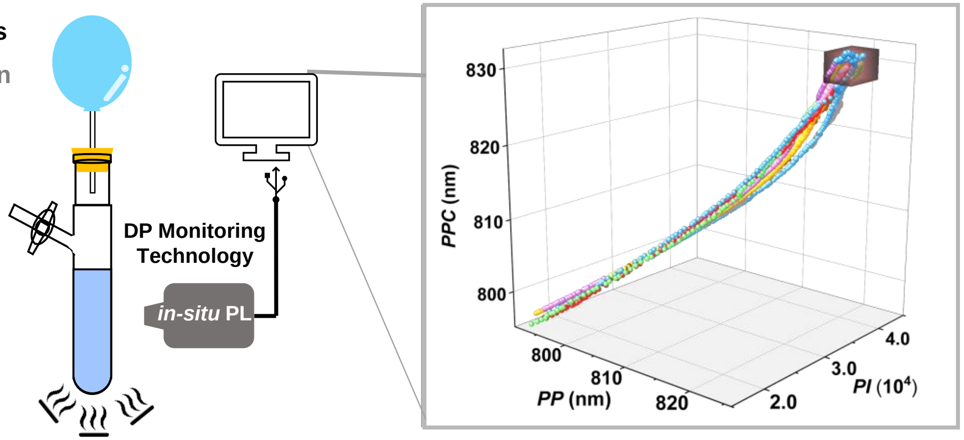
Establishing a correlation between PL spectral parameters and M_W

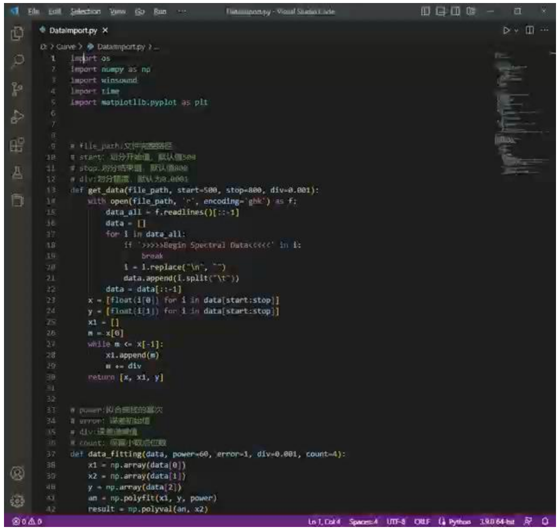
Technical verification: PYT precision synthesis

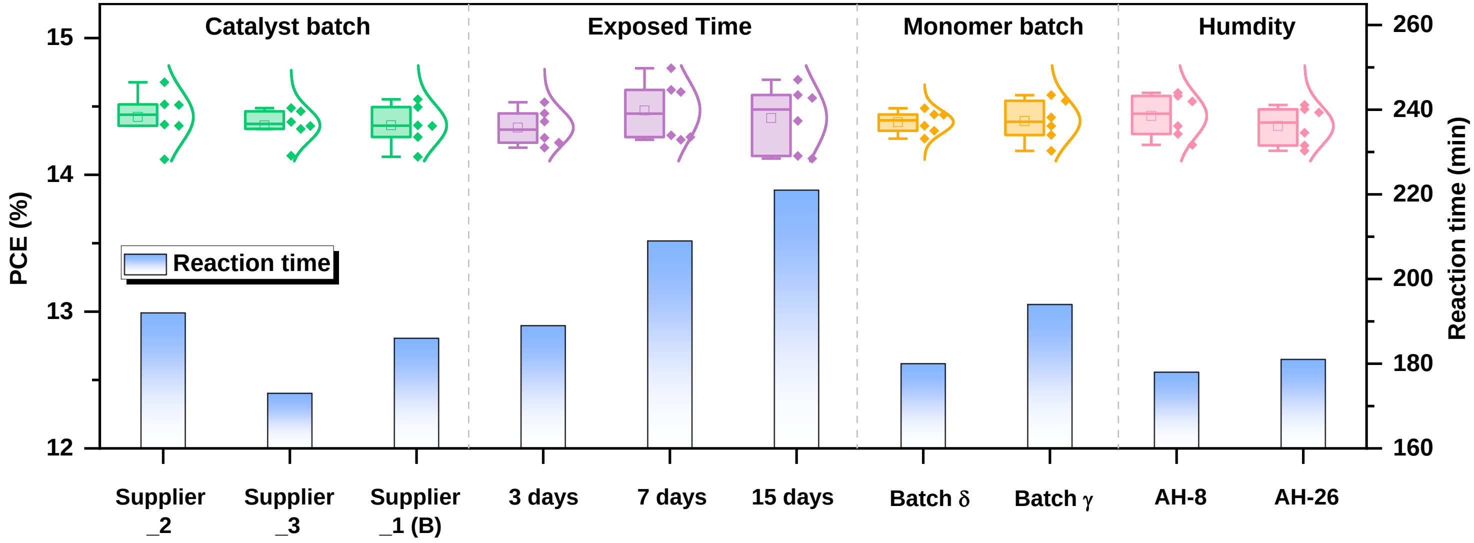
Fixed reaction conditions

- Solution Concentration
- Catalyst Loading
- Solvent
- Temperature

- **Catalyst Batch**
- **Catalyst Aged Time**
- **Monomer Batch**
- **Humidity**



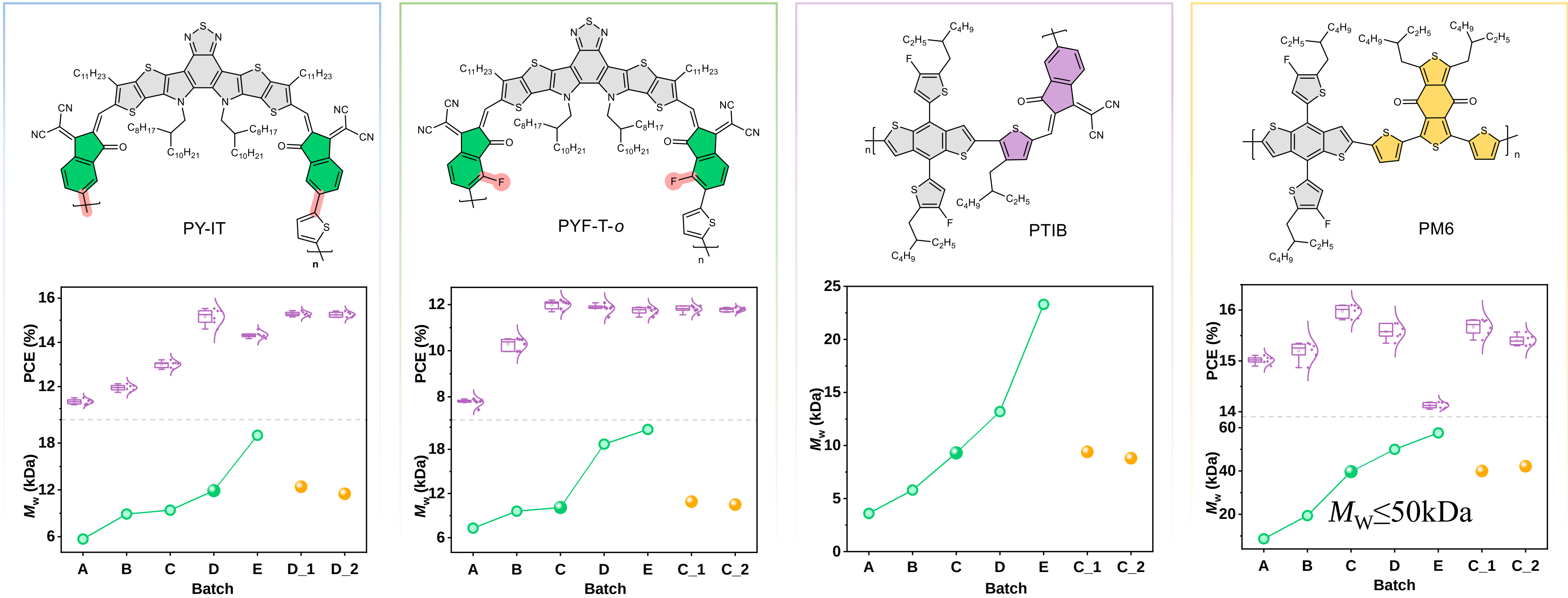




J. Min et. al. Nat. Commun.*, **2024**, *15*, 1248

Technical verification: oligomer precision synthesis

Universality testing based on different P_A materials



PSMA materials
PYT derivatives

D-A copolymer acceptor

D-A copolymer donor

J. Min* *et. al. Nat. Commun.*, **2024**,*15*, 1248

Conclusions

Multi-type strategies to achieve highly stable active layer system

Mechanism

Shed light on the destabilization mechanisms in relation to molecular diffusion coefficients and T_g values

Materials

Developed the PSMA strategy and fabricated efficient and stable all-polymer systems with enhanced phase change temperature

Precision synthesis of low and medium M_W polymers to eliminate batch-to-batch variations and keep device performance

Acknowledgements

Collaborators

Professor Christoph Brabec (FAU)

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Professor Zhiguo Zhang (BUCT)

Professor Xiaotao Hao (SDU)

Professor Haiming Zhu (ZJU)

Professor Yang Yang (ZJU)

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Thank you for your attention!

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