Strategic Non-fullerene Blending Of Ternary Organic Photovoltaics For Morphological And Device Performance Enhancement

NANYANG TECHNOLOGICAL UNIVERSITY SINGAPORE

Presented by Chia Wei Min. Luke

Supervised by Asst Prof, Ng Wei Tat, Leonard & Mr Li Yu Jia

Introduction

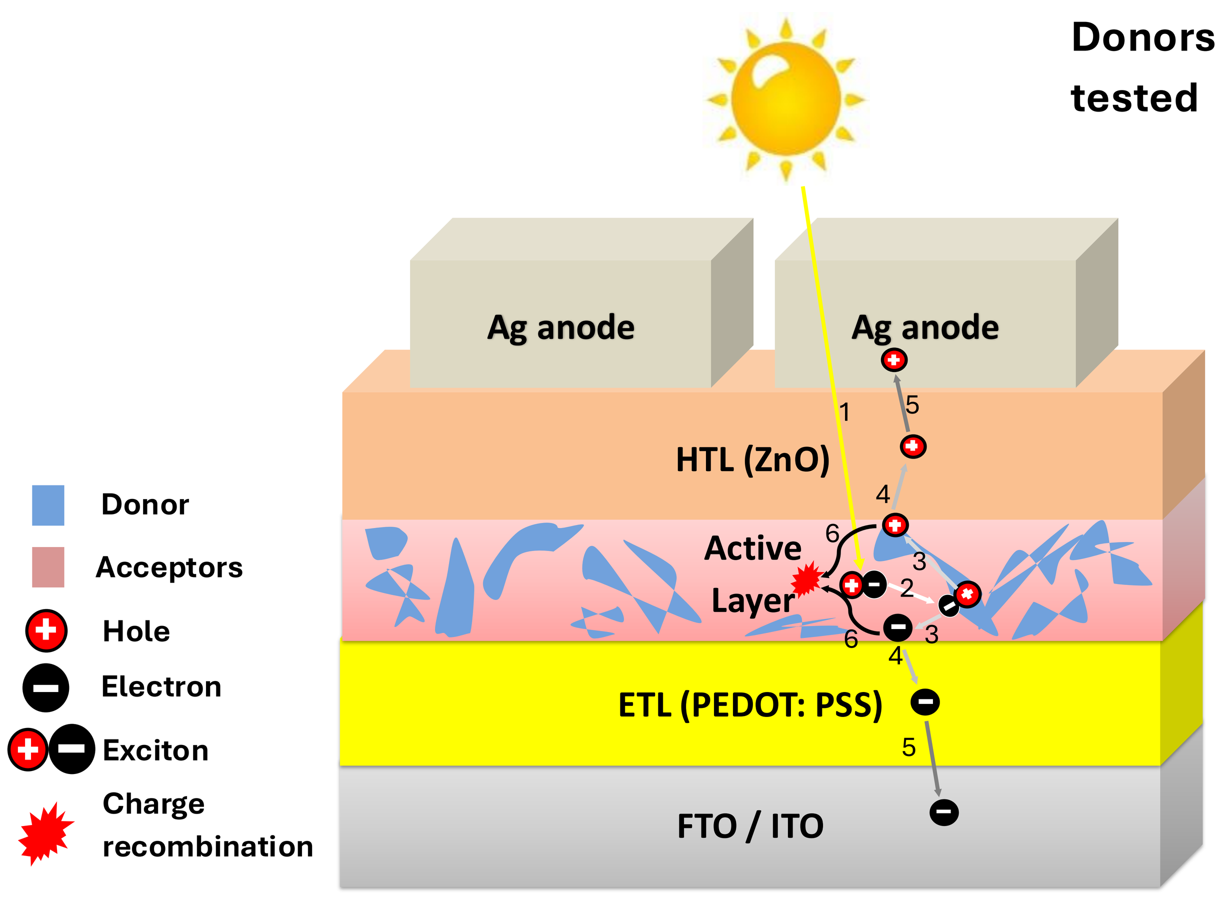
- Organic photovoltaics(OPVs) compared to inorganic PV, have lower environmental impact, are easier to manufacture and have higher absorption coefficients. This allows increased PV generation capacity, reducing climate change.
- Traditional donor and acceptor binary OPVs have drawbacks that ternary devices can solve: wider solar spectrum coverage, better thermodynamic stability reducing phase separation and lower exciton recombination mechanisms.

Research Goal: Investigate ternary D:A:A active layer OPVs devices for enhanced device performance

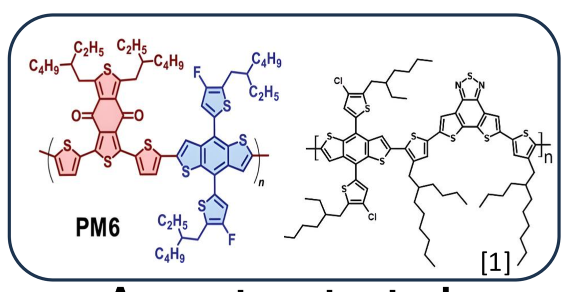
- Create ternary OPV devices based on a 1:1.2 Ratio of different D:A:A blends through spin coating.
- Perform solvent engineering during fabrication on the active layer and judge its performance and processibility.
- Investigate photovoltaic performance (PCE, Jsc, Voc, FF), and its absorption property from UV-Vis characterisation.
- Explain the results through morphological testing (AFM) and crystal structure analysis (GIWAXS).

Methods/steps

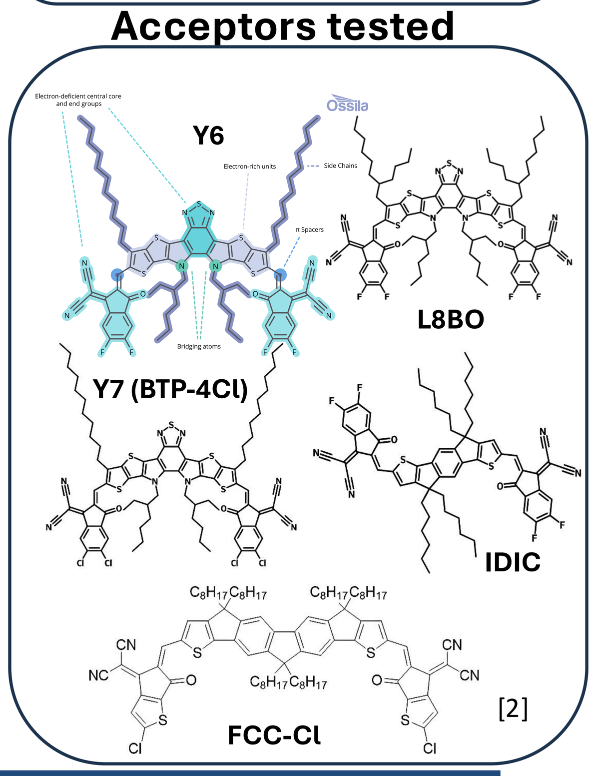
1. Fabricate the inverted OPV devices. Each blend has a ratio of 1:0:1.2, 1:0.3:0.9, 1:0.6:0.6, 1:0.9:0.3, 1:1.2:0.
2. Investigate devices' performance using a solar simulator.
3. Use UV-Vis to investigate how differing ratios have changed absorbance spectra, showing spectra tunability.
4. Using AFM to view each blends' active layer surface to determine uniformity and flatness.
5. Investigating alignment and stacking morphology of conjugated polymer back bone to explain device performance.



Donors tested

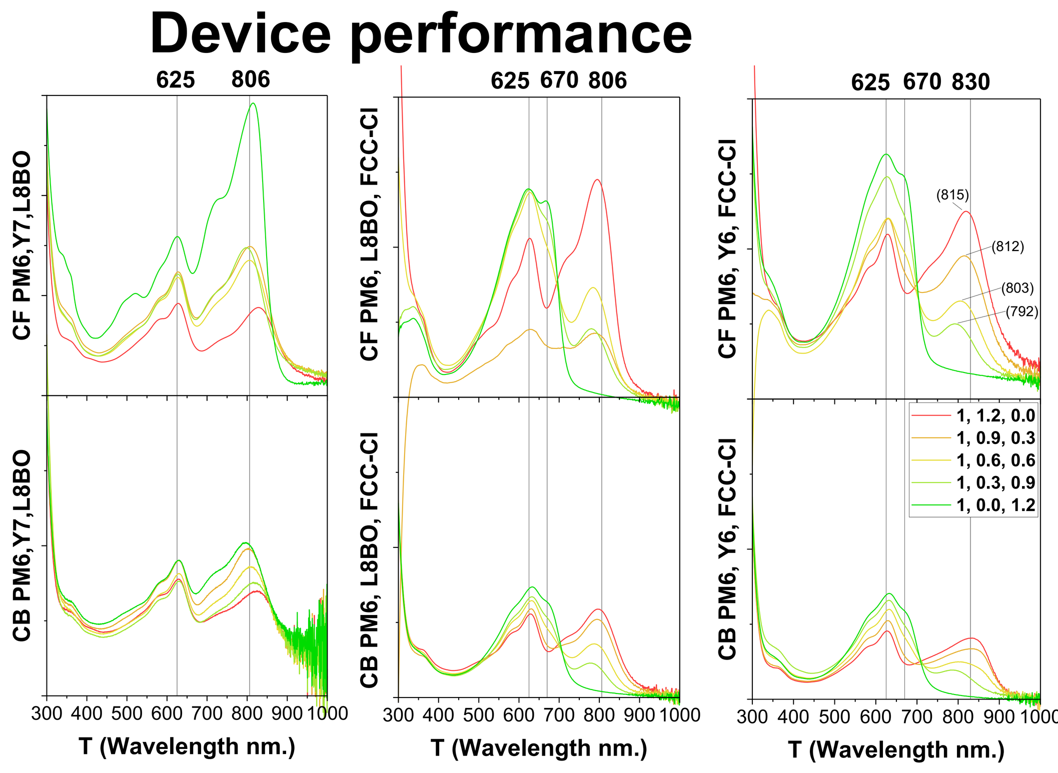


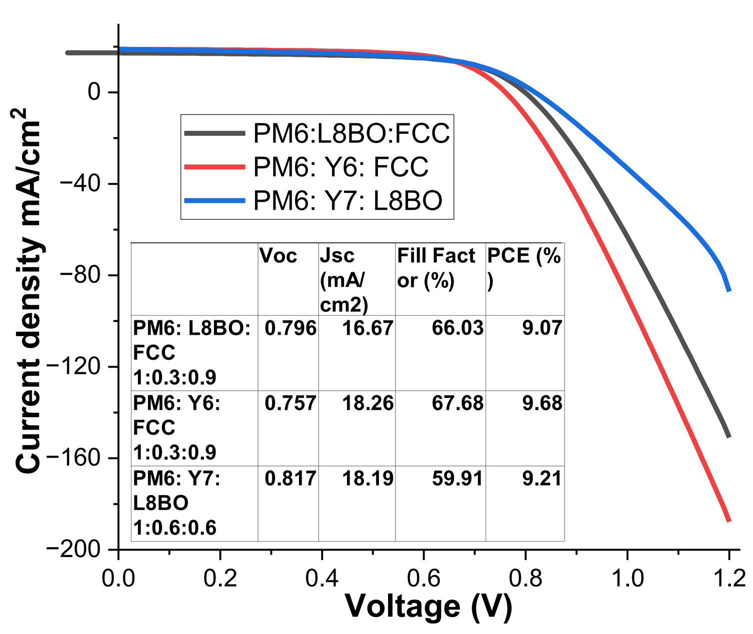
Acceptors tested



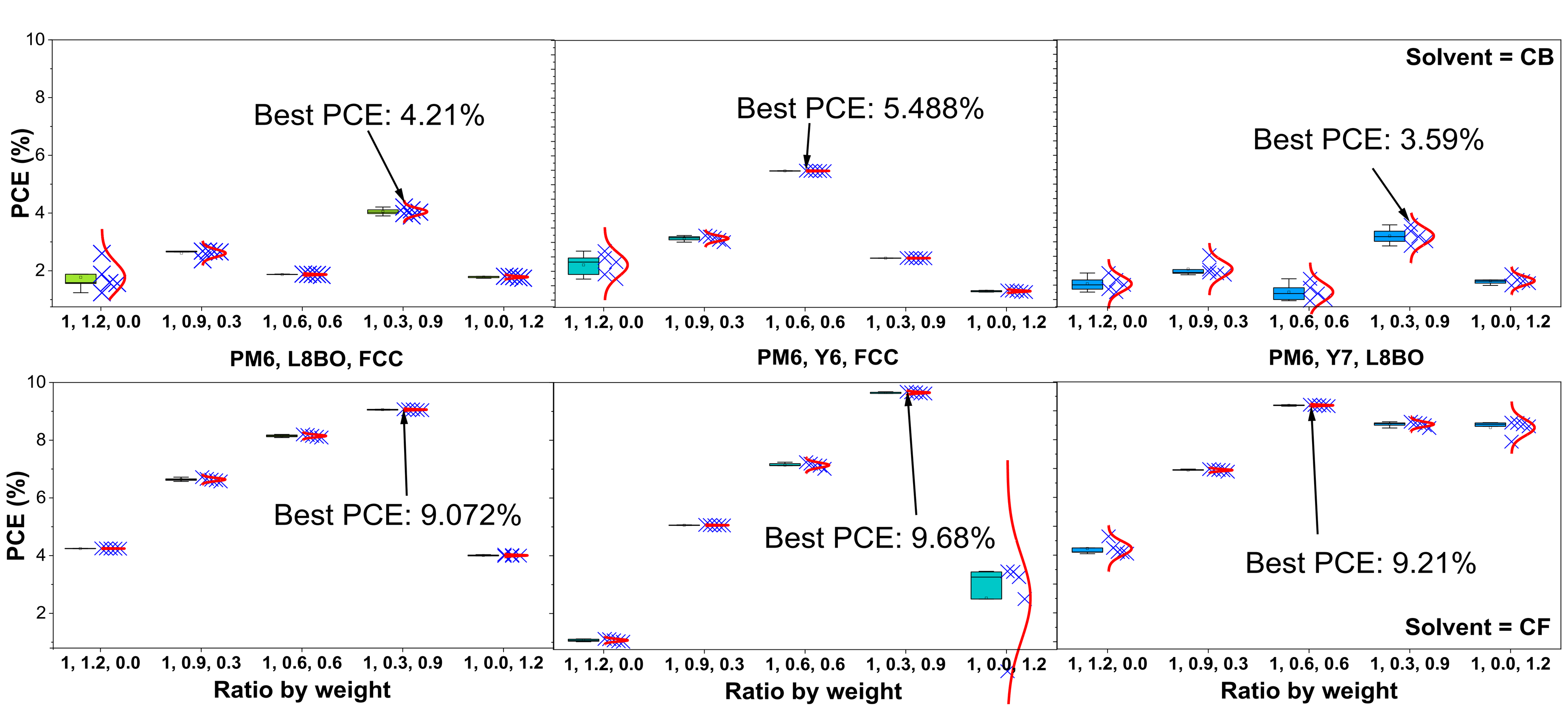
Results and discussion

Device performance





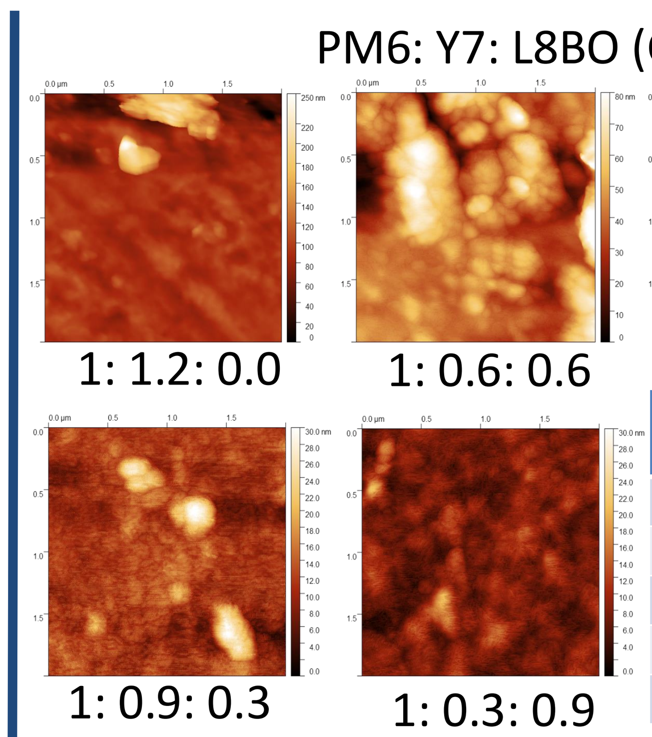
	Voc	Jsc (mA/cm2)	Fill Factor (%)	PCE (%)
PM6: L8BO: FCC 1:0.3:0.9	0.796	16.67	66.03	9.07
PM6: Y6: FCC 1:0.3:0.9	0.757	18.26	67.68	9.68
PM6: Y7: L8BO 1:0.6:0.6	0.817	18.19	59.91	9.21



1. The PCEs of ternary active layer blends above are substantially higher than binary active layer devices
2. Addition of 3rd acceptor widens visible light absorption of active layer
3. Although possessing better processibility, CB has worse PV performance than CF for all blends tested

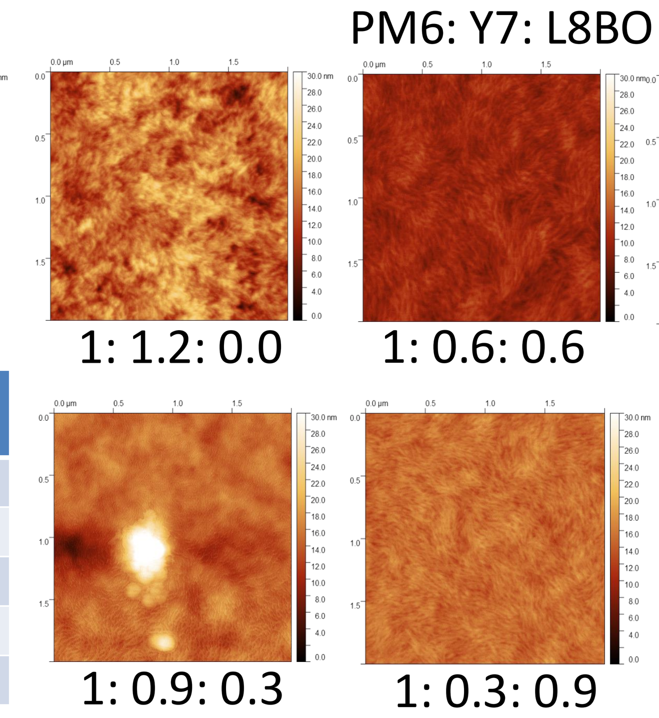
AFM and GIWAXS morphological analysis

PM6: Y7: L8BO (CB)



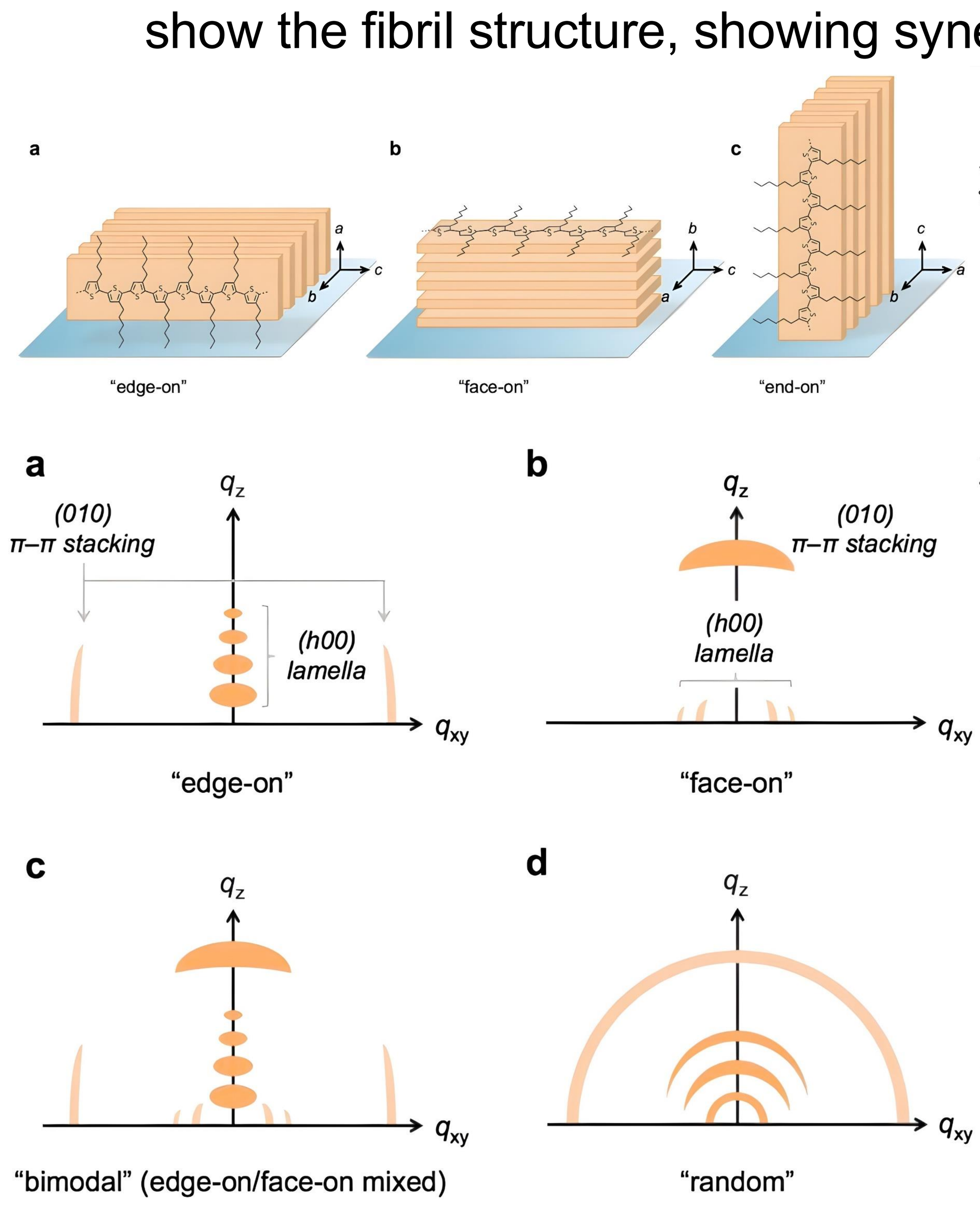
PM6: Y7: L8BO (CB)	Rq (nm)
1: 1.2: 0.0	25.84
1: 0.9: 0.3	2.507
1: 0.6: 0.6	13.65
1: 0.3 : 0.9	4.125
1: 0.0: 1.2	8.437

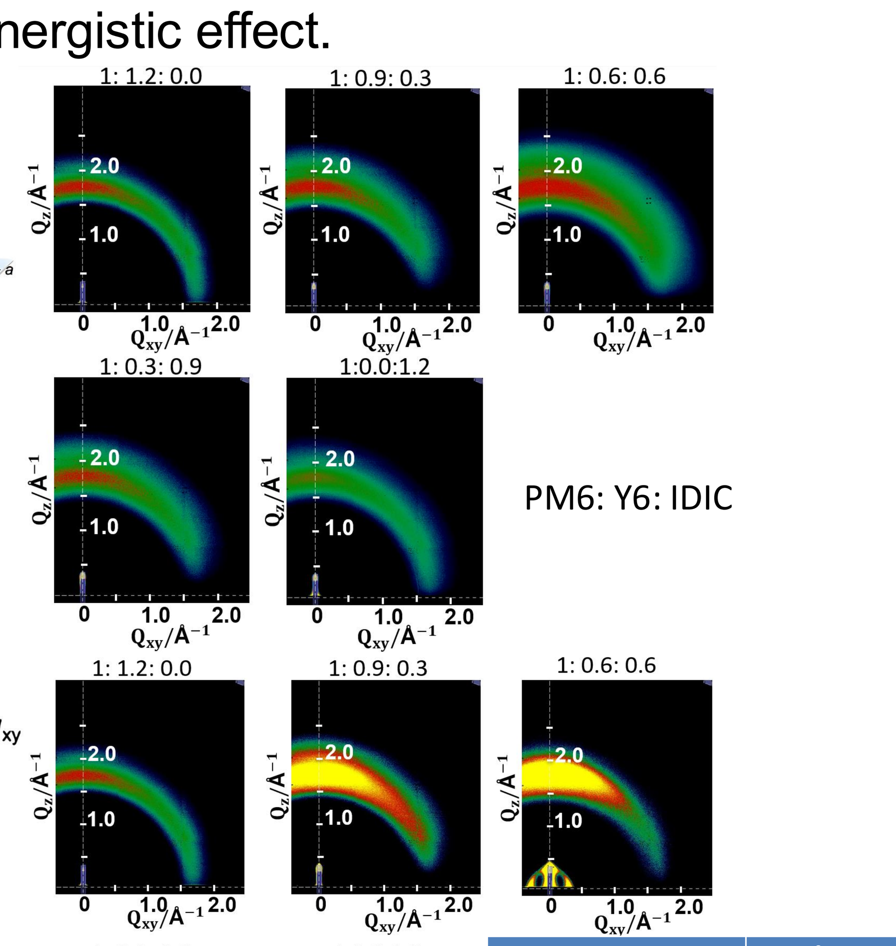
PM6: Y7: L8BO (CF)

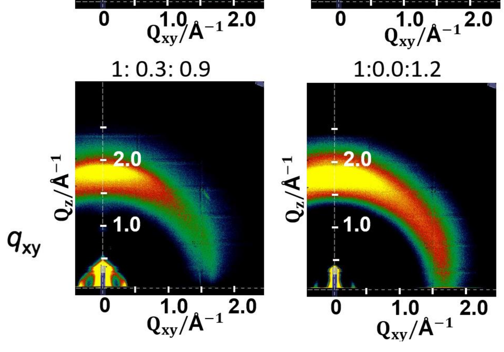


PM6: Y7: L8BO (CF)	Rq (nm)
1: 1.2: 0.0	2.728
1: 0.9: 0.3	3.735
1: 0.6: 0.6	1.261
1: 0.3 : 0.9	1.258
1: 0.0: 1.2	3.033

a) Using CF as solvent induces formation of 2D fibril network structure, which increases charge transport.
b) Using CB as a solvent forms crystals with random orientations with weak π-π stacking.
c) For some blends, like D18-Cl: Y7: L8BO, only ternary active layers show the fibril structure, showing synergistic effect.







PM6: Y6: FCC-Cl	Å^{-1}
Pi-Pi stacking of PM6	1.75 (face-on)
PM6 (100)	0.29
OOP π–π stacking PM6 (010)	1.66
Lamellar stacking	0.27 & 0.43

a) Face-on π-π stacked active layers observed by GIWAXS in PM6:Y6:FCC-Cl shows greatest device performance.
b) Synergistic effect between some acceptors increases stacking alignment, increasing charge transport efficiency

Conclusion

1. Ternary active layer blend on average out performed its binary counterparts.
2. Some acceptors exhibit synergistic effects that causes formation of 2D fibril network and promotes face-on π-π stacking.
3. From our results, although having better processibility, using CB is detrimental to device performance.

Future recommendations

1. Use computational quantum modelling of density functional theory to simulate π-π stacking probability.
2. Fabricate devices in a glove box and using different ETL/HTLs might increase the devices' thermodynamic and photo-stability.

References:

[1] 'Y6 in Solar Cells: Structure, Benefits, Alternatives and Donors', Ossila. Accessed: Mar. 10, 2025. [Online]. Available: https://www.ossila.com/pages/what-are-y6-acceptors
[2] 'PBDB-T-2F (PM6)', Ossila. Accessed: Feb. 16, 2025. [Online]. Available: https://www.ossila.com/products/pbdb-t-2f
[3] I. Osaka and K. Takimiya, 'Backbone orientation in semiconducting polymers', *Polymer*, vol. 59, pp. A1–A15, Feb. 2015, doi: 10.1016/j.polymer.2014.12.066.