**From solution-processed to molecular beam-deposited organic thin films**

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The consensus to propel organic solar cells (OSCs) into a circular economy prioritizes using renewable and abundant materials, weeding out toxic chemicals, following sustainable manufacturing practices, and designing recycling and end-of-life biodegradation routes.[1] Despite this, the synthesis and processing of state-of-the-art materials heavily rely on petrochemical-based ingredients and halogenated solvents for cross-coupling reactions and purification to form optimal morphologies, leading to record performances.[2] We systematically investigate a two-by-two polymer donor and small molecule acceptor (SMA) matrix to unravel the molecular structure-morphology relationship and its impact on the overall OSC performance. Thus, archetypal polymer donors PM6 and PTB7-Th are binarily blended with BTP-eC9 and BTPV-4F-eC9 SMAs to achieve varying morphologies through minor molecular structure differences in SMAs and correlate the morphological features to key device metrics. OSCs based on BTP-eC9 as an acceptor are more resilient to solvent changes across the board and outperform their BTPV-4F-eC9 counterparts when industry-oriented solvents are used. The considerable variation in power output in BTP-eC9 and BTPV-4F-eC9-based OSCs is attributed to the solvent-related over-aggregation or lack thereof,[3] in particular in non-halogenated solvents, that impacts the charge generation, essential for efficient device performance.

At PDI, our primary motivation is to explore the fundamental mechanisms relevant to the molecular structure of the organics and how their effect on the organic film structure impacts device-level performance of photovoltaic cells. The ultimate vision is to establish a structure property relationship across all relevant length scales, i.e. from atomic-scale arrangement of organic molecules at organic-organic but also at organic-inorganic interfaces, their thickness, stacking sequence and other structural parameter at a mesoscale level to decipher the different roles that the various organic molecules, their arrangement, and their interface configurations can have on optoelectronic processes taking place in these heterostructures. We will then also probe structural rigidity and 'device stability' under operating conditions using the newly developed organic molecules that are currently driving the field.

1. Corzo, D. *et al.* High-performing organic electronics using terpene green solvents from renewable feedstocks. *Nat Energy* **8**, 62–73 (2022).
2. Zheng, Z. *et al.* Tandem Organic Solar Cell with 20.2% Efficiency. *Joule* **6**, 171–184 (2022).
3. Fan, H., Yang, H., Wu, Y., Cui, C. & Li, Y. Phenanthrene Treatment for *O* -xylene-Processed PM6:Y6-Based Organic Solar Cells Enables Over 19% Efficiency. *Adv Energy Mater* **15**, (2025).