Moiré superlattices in two-dimensional polymer bilayers

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There has been a growing interest in synthetic, crystalline two-dimensional polymers (2DPs) due to their modular, tailor-made structures and numerous potential applications. The on-surface synthesis of such 2DP monolayers has received a lot of attention. However, the growth of such crystalline films is still poorly understood. So far, most in-situ studies have focused on investigating the lateral bond propagation of the first-layer polymer,[1] while the mechanism governing the formation of subsequent layers remains largely unclear. Study of the monolayer-to-bilayer transition provides further insight into the stacking dynamics involved in the growth of covalent organic frameworks (COFs), which also impacts its pore size and topology.[2]
In this contribution [3], we studied the growth of bilayer 2D boroxine 2D polymers at the solution-substrate interface. In addition to the well-known AA stacking modes, we unveiled large area moiré superlattice patterns arising from a twisted bilayer stacking. Moreover, the choice of ditopic building blocks influences the ratio of twisted to non-twisted stacking populations, and extended moiré-twisted bilayer areas with a common twist angle can be synthesized using asymmetrical building blocks. The specific twist angles observed experimentally consort with twist angle energetics predicted by density functional theory (DFT) calculations.

References

[1] G. Zhan, K. Strutyński, L. Yu, N. Herrmann, M. Martínez-Abadía, M. Melle-Franco, A. Mateo-Alonso and S. De Feyter, Nature. (2022), 603 (7903), 835
[2] Wang, L., Wang, X., Zhao, Z.-L., Wan, L.-J., & Wang, D., Journal of the American Chemical Society (2024) *146*(20), 14079–14085.
[3] Zhan, G., Koek, B., Yuan, Y. *et al. Nature Chemistry,* (2025)

Figures

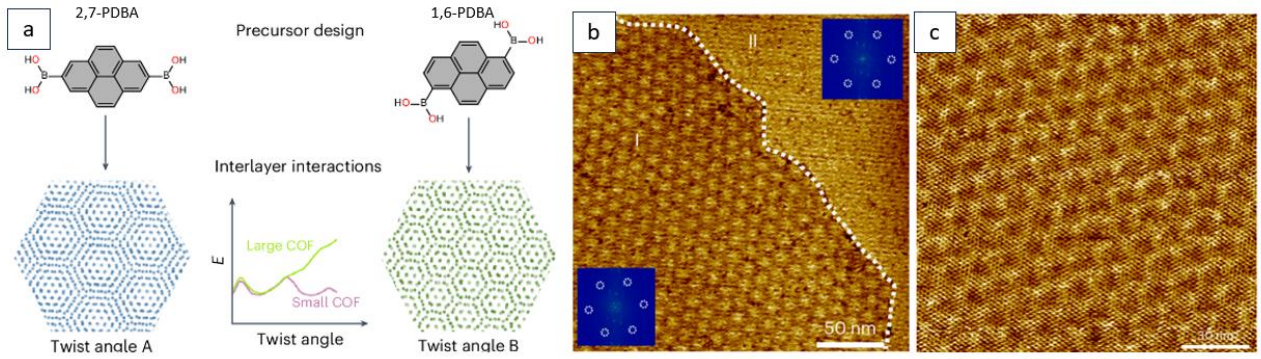

Figure 1: a)scheme showing monomer structure and corresponding moiré patterns; b)STM image of 2.7-PDBA with both moiré and non-moiré domain; c) STM image of 1,6-PDBA showing extended moiré pattern