Atomic lattice reconstruction in twisted transition metal dichalcogenides and arising interfacial ferroelectricity.

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Abstract

In this talk I will review our latest work on twisted TMDs bilayers and discuss atomic reconstruction that occurs when the twist angles are small. For small twist near the 2H stacking, stable 2H domains dominate, with nuclei of a second metastable MM phase. This appears as a kagome-like pattern at θ~1°, transitioning at θ→0 to a hexagonal array large 2H domains. The tunnelling measurements show that such reconstruction creates piezoelectric textures, opening a new avenue for engineering of 2D material properties.
For 3R stacking, a pattern of mirror reflected triangular 3R domains merges, featuring layer-polarized conduction band states caused by lack of both inversion and mirror symmetries. Surprisingly, the lack of inversion symmetry in 3R polytype leads to emergence of out-of-plane ferroelectricity due to layer-asymmetric interband hybridisation. The electrically-polarised domains can be switched by external electric field which opens a new pathway towards optoelectronic devices with memory effect.

References

[1] Weston et al. Nat. Nanotechnol. 2020, 15 (7), 592.
[2] Weston et al. Nat. Nanotechnol. 2022, 17 (4), 390.

Figures

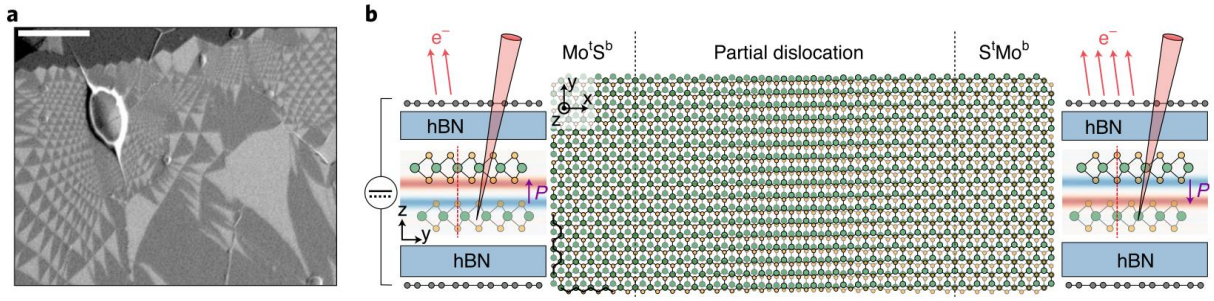

Figure 1: Ferroelectric domains in marginally twisted bilayer MoS_2. **a**, Example of BSECCI acquired on unencapsulated twisted bilayer MoS_2 placed onto a graphite substrate. Light and dark domain contrast corresponds to the two dominant stacking orders referred as Mo_tS_b and S_tMo_b. Scale bar, 1 μm. b, Centre: schematic demonstrating the transition from Mo_tS_b to S_tMo_b with perfectly stacked bilayer regions separated by a partial dislocation. Side panels: the cross-sectional alignment of the MoS_2 monolayers, viewed along the armchair direction, assembled within the double-gated device structure. Colour maps overlayed on top of the TMD atomic schematics show calculated charge density transferred between top and bottom layers.