Atomic reconstruction in twisted TMD interfaces and their electronic properties.

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Twisted heterostructures of two-dimensional crystals offer a broad scope for the design of novel metamaterials. 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 MM metastable phase. This appears as a kagome-like pattern at ~1 degree twist, transitioning below 0.3 degree to a hexagonal array of 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] A. Weston et al. Nat. Nanotechnol. 15, 592-597 (2020)
[2] A. Weston et al. arXiv:2108.06489

FIGURES

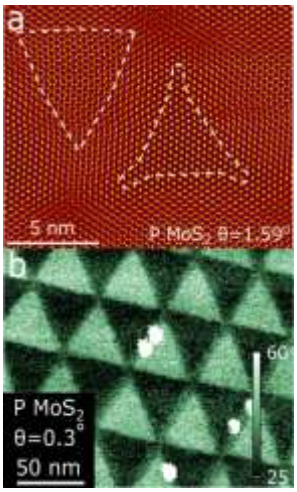

Figure 1: (a) Atomic resolution STEM imaging of the reconstructed lattices in twisted bilayer MoS2 (b)Conductive AMF image of the 3R domain structure indicating layer-polarised electronic wave functions.

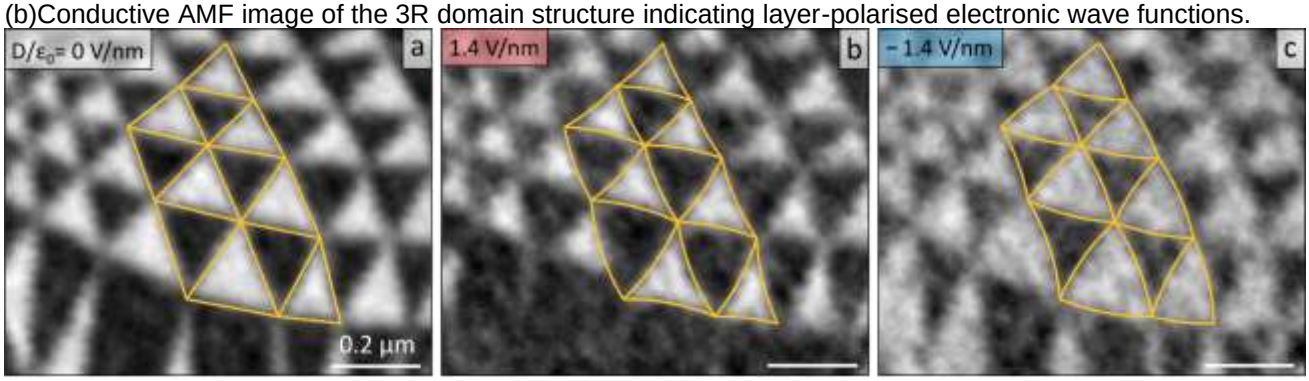

Figure 2: Domain evolution under transverse electric field.