Atomic reconstruction in twisted TMD interfaces and their electronic properties

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Van der Waals heterostructures form a massive interdisciplinary research field, fueled by the rich material science opportunities presented by layer assembly of artificial solids with controlled composition, order and relative rotation of adjacent atomic planes. I will present our atomic resolution transmission electron microscopy and multiscale modeling to show that the lattice of MoS_2 and WS_2 bilayers twisted to a small angle, $\theta < 3^{\circ}$, reconstructs into energetically favorable stacking domains separated by a network of stacking faults. For crystal alignments close to 3R stacking, a tessellated pattern of mirror reflected triangular 3R domains emerges, separated by a network of partial dislocations which persist to the smallest twist angles. Scanning tunneling measurements show that the electronic properties of those 3R domains appear qualitatively different from 2H TMDs, featuring layer-polarized conduction band states caused by lack of both inversion and mirror symmetry. In contrast, for alignments close to 2H stacking, stable 2H domains dominate, with nuclei of an earlier unnoticed metastable phase limited to ~ 5nm in size. This appears as a kagome-like pattern at $\theta \sim 1^{\circ}$, transitioning at $\theta \rightarrow 0$ to a hexagonal array of screw dislocations separating large-area 2H domains.