Stacking Ferroelectricity and Band-Edge Physics in 2D Semiconductors

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Recently, experiments and theory have established an unconventional route to ferroelectricity in stacked van der Waals layers: when two layers are assembled in a non-centrosymmetric (inversion-breaking) registry, weak interlayer hybridisation generates an out-of-plane polarisation [1]. The magnitude and sign of this polar response are set by the lateral stacking offset (registry), turning registry into a "lever" for electric-field tuning of ferroelectric and other order parameters in bilayer and multilayer devices.

In this talk, I highlight our recent work, identifying uses and properties of registry-driven FE. (i) **Marginal twist and reconstruction**: in TMD heterostructures, relaxation into commensurate stacking domains reshapes excitonic and electronic localisation landscapes and can yield self-organised quantum dots [2,3]; I will also discuss how analogous reconstruction in metallic $NbSe_2$ can tune charge-density-wave and superconducting order [4]. (ii) **Interface electronics in bulk 3R-TMD FEs**: we have predicted that twin boundaries in 3R-TMDs can host 2D electron/hole gases with stable photo-doped density $n^* \sim 8\times10^{12}$ cm^{-2} [5]. At "magic" twist angles, commensurability between n^* and the moiré pattern can promote strongly correlated states, such as Wigner crystals [1,2]. (iii) I will also review our **high-throughput DFT** efforts to identify vdW-ferroelectric candidates and map how pressure, surface charging, and internal interfaces can regulate the polar response [6]. (iv) **Stacking-enabled multiferroicity**: stacking order provides a route to engineer multiferroic functionality, including controllable spin splitting and stacking-dependent non-relativistic spin splitting (NRSS) for prospective spintronic applications.

References

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Figures

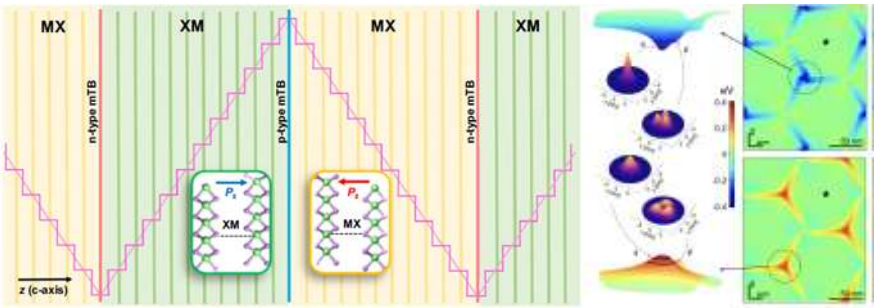

Figure 1: (**Left**) Mirror twin boundaries in ferroelectric TMDs. Schematic of mirror twin boundaries separating adjacent ferroelectric domains in 3R-TMDs (with MX- and XM-stacking). (**Right**) Conduction and valence band edge profiles in marginally twisted AP-$MoSe_2$/WSe_2