First-Principle of Ferroelectric Interface Quantum Wells in 2D TMDs

Xue Li
James G. McHugh, Isaac Soltero, Vladimir I. Fal'ko
Department of Physics and Astronomy, University of Manchester, Oxford Road, Manchester, M13 9PL, United Kingdom
National Graphene Institute, University of Manchester, Booth St. E., Manchester, M13 9PL, United Kingdom
Vladimir.Falko@manchester.ac.uk

Ferroelectricity emerging in stacked two-dimensional (2D) transition metal dichalcogenides (TMDs) provides an intrinsic route to engineer electronic properties in layered materials.[1,2] In rhombohedral (3R) TMDs, the lack of inversion symmetry leads to pronounced interlayer charge redistribution, giving rise to robust out-of-plane ferroelectric polarization and strong internal electric fields.[3] These built-in fields naturally confine electrons and holes into atomically thin quantum wells at interfaces between domains of opposite polarization, known as mirror twin boundaries (mTBs).[4,5] We combine first-principles density functional theory (DFT) with a self-consistent Thomas-Fermi approach to establish a predictive framework for polarization-driven quantum confinement at ferroelectric twin boundaries in van der Waals TMDs, enabling systematic evaluation of carrier accumulation, confinement stability, and external tunability across a broad materials space (Figure 1). This work establishes ferroelectric mTBs as a programmable internal interface platform for hybrid integration, enabling built-in fields to define and tune quantum-confined channels relevant to nanoscale optoelectronic, photonic, and quantum device architectures, while reducing reliance on external gating and complex heterostructures.

References

[1] Vizner Stern, M.; Waschitz, Y.; Cao, W.; Nevo, I.; Watanabe, K.; Taniguchi, T.; Sela, E.; Urbakh, M.; Hod, O.; Ben Shalom, M. Science, 372, (2021) 1462–1466.
[2] Weston, A.; Castanon, E. G.; Enaldiev, V.; Ferreira, F.; Bhattacharjee, S.; Xu, S.; Corte-León, H.; Wu, Z.; Clark, N.; Summerfield. Nat. Nanotechnol. 17, (2022) 390–395.
[3] Wang, X.; Yasuda, K.; Zhang, Y.; Liu, S.; Watanabe, K.; Taniguchi, T.; Hone, J.; Fu, L.; Jarillo-Herrero, P. Nat. Nanotechnol. 17, (2022) 367–371.
[4] McHugh J, G.; Li, X.; Soltero, I.; Falko, V. Nat. Commun. 15, (2024) 6838.
[5] Li, X.; McHugh J, G.; Falko, V. Acad. Nano: Sci., Mater., Technol. 2 (2025).

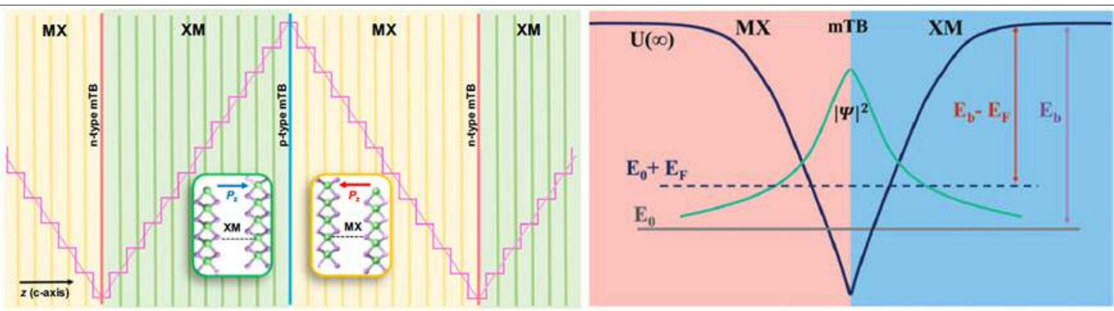

Figure 1: (Left) Mirror twin boundaries in ferroelectric TMDs. Schematic of mirror twin boundaries separating adjacent ferroelectric domains in 3R-TMDs (with MX- and XM-stacking). (Right) Schematic illustration of the electro-static potential profile across a mTBs, and the green curve displays the probability density ($|\Psi(z)|^2$) of accumulated carriers. The black curve is the potential profile in triangular well.