Moiré Band Engineering in Twisted Trilayer 2D Materials: From Graphene to TMDs

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Abstract (Century Gothic 11)

We present a comparative theoretical study on lattice relaxation and electronic structures in two distinct families of twisted trilayer systems: graphene and transition metal dichalcogenides (TMDs). In twisted trilayer graphene, we uncover a complex relaxation pattern forming a patchwork of moiré-of-moiré domains, where moiré patterns from adjacent layer pairs become locally commensurate [1]. The resulting electronic structures strongly depend on the twist configuration: helical and alternating stacks. In particular, helical trilayers host one-dimensional topological boundary states between distinct Chern insulating domains.

In twisted trilayer TMDs such as WSe_2, the relaxation similarly leads to the formation of the domain structures, but with a crucial difference in the resulting electronic properties [2]. In twisted trilayer TMDs, the electronic structure is primarily governed by the intralayer moiré potential rather than interlayer hybridization, leading to characteristic layer-polarized states near the valence band edge. A key feature is that moiré potentials from both top and bottom layers superpose on the middle layer, effectively doubling the potential depth. In helical trilayers, this mechanism generates a Kagome lattice potential that gives rise to flat bands characteristic of Kagome physics, while in alternating configurations, the enhanced potential confinement forms deep triangular quantum wells. Furthermore, we demonstrate that a moderate perpendicular electric field can switch the layer polarization near the valence band edge, providing an additional degree of tunability. It also enables tuning of the hybridization between orbitals on different layers, allowing for the engineering of diverse and controllable electronic band structures. Our study demonstrates how trilayer stacking enables a new degree of control over moiré physics, going beyond the possibilities of bilayer systems.

References

[1] N. Nakatsuji, T. Kawakami, and M. Koshino, Phys. Rev. X 13, 041007 (2023).
[2] N. Nakatsuji, T. Kawakami, and M. Koshino, arXiv:2504.20449 (2025).