Complete symmetry indicators classification of moiré materials

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Thesis possibility after internship: Yes, requires an official application to UofT's graduate program.

Background:

Moiré materials are engineered systems formed by stacking two-dimensional crystals with a slight twist (Fig. 1) or lattice mismatch, creating long-wavelength interference patterns known as moiré superlattices[1]. These structures dramatically alter electronic interactions, enabling the emergence of strongly correlated states in otherwise weakly interacting materials. They offer tantalizing prospects as quantum simulators, having already achieved analogs of high-temperature superconductors and (topological) fractional quantum Hall states.

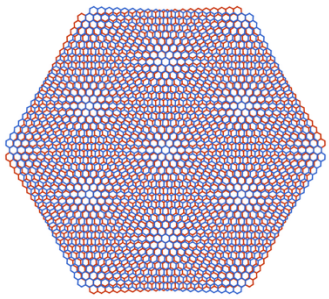

Figure 1: moiré pattern created by two honeycomb latice twisted by a few degrees.

A central question arises: *Which material should you choose, and which moiré configuration should you engineer to reach a specific phase of interest?* This is where the curse of dimensionality strikes—the design space of moiré systems is vast, encompassing countless combinations of materials, twist angles, and external conditions.

There is, however, an elegant way out. Recent advances in *perturbative symmetry indicators* provide a powerful framework for classifying moiré bands across the entire design space. By leveraging symmetry-based diagnostics and perturbation theory[2], we can predict correlated phases without exhaustive numerical simulations, enabling a high-throughput approach to identify promising candidates for quantum technologies[3].

Project:

The goal of the proposed internship is to complete the classification of perturbative symmetry indicators for moiré systems – an ambitious task grounded in elegant mathematics with direct impact on material selection and discovery when combined with large-scale numerical screening of databases. The mathematical theory for the project relies on elementary band representations of periodic systems. In essence, it uses group-theoretic methods at all momentum high-symmetry points to determine the representations carried by the system. By adiabatically "gluing" these representations in momentum space, one can distinguish the nature of the system: Is it topological? Can it be described by localized atomic orbitals? If so, where should these orbitals be located in real space?

Your role will be to *develop the full mathematical framework to apply this theory systematically to any pair of stacked or twisted materials*. Once this classification is complete, we will be able to perform inexpensive numerical calculations to identify which materials are best suited for realizing topological phases.

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[1] The term "moiré" was popularized to refer to a particular silk fabric invented in Lyon.

[2] Crépel, V., & Cano, J. (2025). Efficient prediction of superlattice and anomalous miniband topology from quantum geometry. *Physical Review X*, *15*(1), 011004.

[3] Nakatsuji, N., Cano, J., & Crépel, V. (2025). High-throughput discovery of moiré homobilayers guided by topology and energetics. *arXiv preprint arXiv:2512.15851*.