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Electronic properties of moire superlattice bands in layered two dimensional materials[1]

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When atomically thin two-dimensional materials are layered they often form incommensurate non-crystalline structures that exhibit long period moiré patterns when examined by scanning probes. In this talk, I will present a theoretical method which can be used to derive an effective Hamiltonian for these twisted van der Waals heterostructures using input from ab initio calculations performed on short-period crystalline structures. I will argue that the effective Hamiltonian can quantitatively describe the electronic properties of these layered systems for arbitrary twist angle and lattice constants [1-2]. Applying this method to the important cases of graphene on graphene and graphene on hexagonal-boron nitride, I will present a series of experimentally observable quantities that can be extracted from their electronic structure, including their density of states and local density of states as a function of twist angle, and compare with available experiments.

[1] Moire bands in twisted double-layer graphene, R. Bistritzer and A. H. MacDonald, PNAS 108 (30), 12233 (2011).
[2] Ab initio theory of moire bands in layered two-dimensional materials, J. Jung, A. Raoux, Z. H. Qiao and A. H. MacDonald, (submitted).

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