Modeling and computation of electronic properties in incommensurate stacks of $2D$ materials

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Abstract: Weak van der Waals interactions between $2D$ materials layers do not impose limitations on integrating highly disparate materials such as graphene, hexagonal boron nitride and many others. This is both a blessing, allowing the realization of many more configurations, and a curse from a modeling perspective due to the loss of periodicity. Unusual geometries appear at the atomic-scale, such as lattice mismatches, twist angles and Moire patterns, providing new challenges for our fundamental understanding.

We discuss how tight-binding electronic structure models for such assemblies fall within the framework of abstract C^*-algebras introduced by Bellissard for general aperiodic condensed matter systems. We present efforts towards an effective direct implementation of these abstract objects, and the design of new algorithms for computing Kubo formulae associated with macroscopic observables such as the conductivity. This leads to a completely new numerical framework allowing to perform calculations outside the scope of usual methods involving finite-volume periodic approximants.