Twisted bilayer graphene: from DFT to moiré-scale models

Eric Cancès
Ecole des Ponts and Inria Paris

Abstract

This talk will deal with with the mathematical derivation of effective moiré-scale electronic structure models for twisted bilayer graphene from Density Functional Theory (DFT). In the first part of the talk (joint work with Louis Garrigue and David Gontier), I will present a simple formal derivation and compare the resulting moiré-scale model with the Bistritzer-MacDonald model. In the second part of my talk (work in progress with Long Meng), I will discuss a semiclassical formulation of this problem.