Twistronics: electronic transport with a twist

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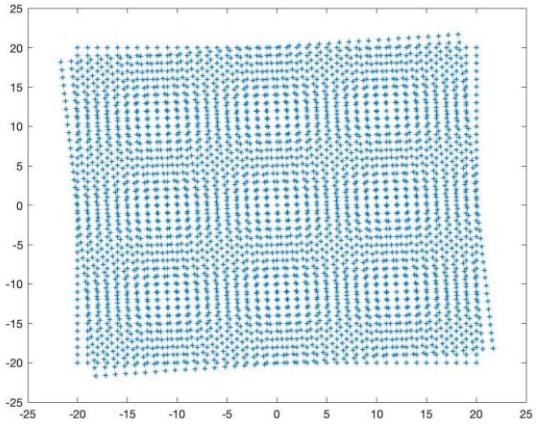
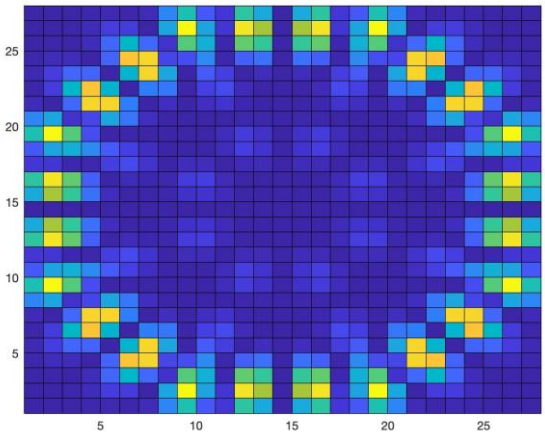
Twistronics is a nascent area concerned with what happens if we take two 2d materials bonded together and twist them through an angle relative to each other. Aside from the fascinating geometrical problem - the formation of moire patterns (picture below) - these novel structures exhibit a host of exciting electronic properties (and hence the term twistronics). They can become completely insulating or superconducting, and this breathtaking wealth of behaviour is controlled by a single parameter: the twist angle.



This is ultimately a tough many-body problem, where both electron-electron and electron-phonon interactions have to be taken into account. However, valuable insight into the nature of the quantum electronic states (example below) in such systems can be gained through simple and tractable electronic models, such as the tight-binding model.



This PhD project builds on an exciting MSci modelling project, in which we set up tight-binding simulations of twisted bilayers and got as far as calculating their conductance. Our next task is two-fold: extending the tight-binding model to more realistic atomic orbital basis sets and adding screening. The latter is in general very hard. Our first port of call will be mean-field methods, akin to LDA in DFT, to reinstate electron-electron interactions and their effect on the bonding and electronic properties of the system.

In our group – the Centre for Quantum Materials and Technologies – we enjoy lively interactions between theory and experiment. These links will be expanded in this project, to gain an understanding into twisted ferroelectric interfaces, where we have world-leading research capability. The project will combine pen and paper theory with computational work, which can potentially become very demanding. To this end we will use the University HPC facilities, and appropriate training will be undertaken early on. If you have a taste for theory and computer simulation with immediate real-life applications, this is the project for you!