Abstract

We characterize the topology and simulate the longitudinal and Hall conductivity of multilayers of graphene encapsulated with hexagonal boron-nitride [1-3]. These systems host multiple moire patterns with different spatial ranges. The moire superlattice is formed by lattice mismatch and relative twist angles. To atomistically simulate these systems is very challenging since the superlattice size must be very large to capture the low energy features. We develop linear scaling algorithms to be able to simulate the longitudinal conductivity as well as the Hall conductivity. Furthermore, when placed under a magnetic field, the system develop topologically non-trivial gaps. We are able to characterize the topology by computing the Chern number with our linear-scaling method [4]. Since our methods are based on real-space, we can continuously tune the twist angle of each layer.

References


Figures

Figure 1: Graphene onsite potential correction coming from a) top and b) bottom hBN layers, and c) composition of both.

Figure 2: Longitudinal conductivity for graphene encapsulated with hBN with small twist angles.