Exploiting Moiré Effects to Control Functionality of Twisted Bilayer Graphene

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Recent studies have established synthesis protocols to enable twisting of bilayer graphene to change the stacking order, thereby controlling the resulting moiré pattern. Due to the moiré, electrical and transport properties of the twisted bilayer graphene are found to be strongly-dependent on the twist angle, thus yielding a new class of low-dimensional carbon system. Interestingly, the periodic moiré networks also correspond to highly localized non-uniform strain field, resulting from van der Waals interaction between these layers. It has been shown that the relative twist angle between graphene bilayers can introduce topological defects that change the momentum phase-space, producing strong correlations in electron-electron interactions. This talk will focus on the connection between electronic structure and the underlying mechanics of twisted bilayer graphene with the help of large scale interatomic force-field and first principles-based atomistic simulations. The novel physical properties and their tunability arising from such systems will be discussed.