Phonon Linewidths in Twisted Bilayer Graphene near Magic Angle

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Electron-phonon interactions play a crucial role in the transport properties of twisted bilayer graphene (TBG), particularly in the vicinity of the magic angle, where exotic electronic phenomena are observed. However, theoretical calculations of electron-phonon interactions in TBG are computationally challenging due to the large number of atoms in the moiré supercell.

In this work, we present a computational study of the phonon linewidths in TBG arising from electron-phonon interactions and anharmonic effects using an atomistic tight-binding model. Our model incorporates the effects of Hartree interactions and distance-dependent transfer integrals approximated using the Slater-Koster formalism. The force constants for the phonon calculations are generated from classical force fields that are used to model the interatomic interactions. Additionally, we account for the effects of phonon-phonon interactions on the linewidths by computing the mode-projected velocity autocorrelation function from classical molecular dynamics.

Our findings show both electron-phonon and anharmonic effects have a significant impact on the linewidth of the G mode. Further, we predict a splitting of the G mode due to the modulation of the moiré potential, which can be detected in experiments. We analyze the spatial origins of these splits and look at the contributions from each high symmetry stacking region.