

Bilayers with a small angular twist: non-adiabatic dynamics in the vicinity of a domain wall

Authors: Shaswati Mandal, Piotr Chudziński

Affiliation: Institute of Fundamental Technological Research of the Polish Academy of Sciences

Abstract: For hexagonal bilayers at the smallest angular twist in between the layers, the resulting Moiré superlattice leads to the emergence of the following spatial pattern: large regions of Bernal stacking separated by narrow frustrated regions that we shall call *domain walls*. Domain walls in such twisted bilayers host strong structural and electronic inhomogeneities that fundamentally alter electron-phonon interactions. In these regions, these spatial variations have a profound impact on how electrons couple to lattice vibrations (phonons) as they are capable of driving the interaction into a non-adiabatic regime. We employ the Effective Correlated Electron-Ion Dynamics equations of motion and develop a framework to model the position-dependent electron-phonon interaction. We are able to study its impact near the domain wall, in particular extract quantitatively the strength of non-adiabaticity. Our analysis highlights the crucial role of anharmonic potentials, which enhances the coupling strength and amplifies non-adiabatic dynamics. In the future, our findings will provide new insight into how local electron-phonon correlation may shape the collective behavior observed in Moiré bilayers, such as superconductivity, correlated insulating phases, etc.