PHYSICS INSIDE THE MOIRE STRUCTURE

Shaswati Mandal[1], Piotr Chudziński[2]

Department of continuum mechanics and nanostructures, Institute of Fundamental Technological Research of the Polish Academy of Sciences
smandal@ippt.pan.pl

For hexagonal bilayers at the smallest angular twist angle between the layers, the resulting Moiré superlattice leads to the emergence of a spatial pattern characterized by large regions of Bernal stacking separated by narrow, frustrated regions that we shall refer to as *domain walls*. Domain walls in such twisted bilayers host strong structural and electronic inhomogeneities that fundamentally alter electron-phonon interactions. In these regions, the 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 correlated electron-ion (ECEID) equations of motion and develop a framework to model the position-dependent electron-phonon interaction. We can study its impact near the domain wall, in particular, and 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 insights into how local electron-phonon correlations may shape the collective behavior observed in Moiré bilayers, such as superconductivity, correlated insulating phases, etc.

Keywords: ECEID- Effective Correlated Electron-Ion Dynamics, Moiré patterns