Lattice dynamics in low-angle twisted bilayer graphene

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Twisted bilayer graphene is created by slightly rotating the two crystal networks in bilayer graphene with respect to each other. [1-4] For small twist angles, the material undergoes a self-organized lattice reconstruction, leading to the formation of a periodically repeated domain. The resulting superlattice modulates the vibrational [1,3] and electronic structures [4] within the material, leading to changes in the behavior of electron–phonon coupling and to the observation of strong correlations and superconductivity.

In this talk, I will report on the phonon spectra of twisted bilayer graphene (tBLG) that were computational analyzed for a series of 692 twisting angle values in the [0, π/6] range. The evolution of the phonon bandstructure as a function of twist angle is examined using a band unfolding scheme where the large number of phonon modes computed at the Γ point for the large moiré tBLG supercells are unfolded onto the Brillouin Zone (BZ) of one of the two constituent layers. In addition to changes to the low-frequency breathing and shear modes, a series of well-defined side-bands around high-symmetry points of the extended BZ emerge due to the twist angle-dependent structural relaxation. I will also review how these results have been confirmed experimentally in collaboration with the group of Ado Jorio: Observations of the crystallographic structure with visible light are made possible by the nano-Raman technique, which reveals the localization of lattice dynamics, with the presence of strain solitons and topological points causing detectable spectral variations.

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FIGURES

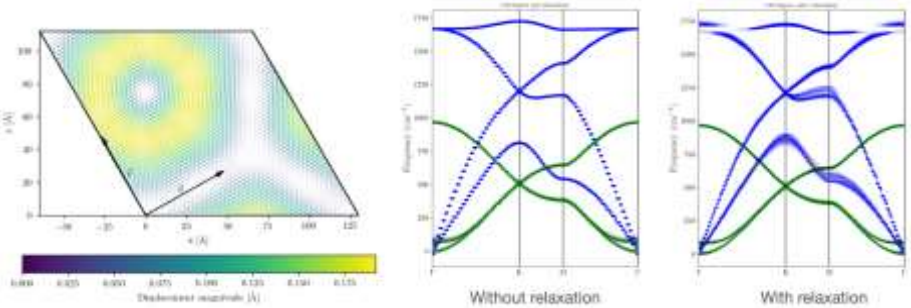

Figure 1: Crystal field due to reconstruction in moiré pattern (top) and unfolded phonon bandstructure with and without full atomic reconstruction. Adapted and reproduced from Ref. [3].