Phonon Dynamics in Reconstructed Twisted Homo and Hetero bilayer System

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Abstract:

Twist angle engineering in van der Waals homo and hetero bilayers introduces profound modifications in their electronic, optical and mechanical properties due to lattice reconstruction. In these systems, the interlayer coupling and atomic rearrangement strongly depend on the twist angle, leading to the formation of periodic moiré superlattices. At small twist angles, significant lattice relaxation results in the emergence of domain structures separated by one-dimensional soliton networks, influencing electronic band structures and phonon modes. Here we systematically investigate the impact of lattice reconstruction on phonon renormalization in twisted bilayer graphene (TBLG, homo) and graphene-hBN moiré superlattices(hetero). In TBLG, we observe the evolution of the G peak, including broadening, splitting, and the emergence of additional peaks in the small angle range 0.3 to 1 degree, attributed to moiré modified phonon interactions. At large twist angles, the peaks gradually merge back into a single feature, reflecting the reduced impact of lattice reconstruction. Similarly, in hBN graphene moiré superlattices, we detect moiré induced Raman peaks above and below the G peak, while the central G peak remains largely invariant to twist angle variation. Our theoretical calculations link these modes to distinct stacking regions, establishing a clear connection between twist angle, lattice reconstruction, moiré phonons, and interlayer coupling, with implications for phonon, optoelectronic, and thermal control in future van der Waal heterostructures.

References

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Figure 1: Evolution of the positions of multiple resonant peaks near the G mode as a function of twist angle in twisted bilayer graphene (TBLG). A pronounced peak splitting appears at intermediate twist angles, where lattice reconstruction is strongest, while at larger twist angles the features progressively merge back toward a single peak.