Phonon Dynamics in Reconstructed Twisted Graphene heterostructures

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Abstract:

Twist-angle engineering in van der Waals homo and hetero-bilayers can dramatically reshape their electronic, optical, and mechanical responses by driving lattice reconstruction. Because interlayer coupling and atomic registry depend sensitively on the relative rotation, twisting generates periodic moiré superlattices whose local stacking evolves with angle. At small twist angles, strong lattice relaxation produces reconstructed domains separated by one-dimensional soliton networks, which in turn modify the band structure and renormalize phonon modes.

Here, we systematically probe how lattice reconstruction governs phonon renormalization in twisted bilayer graphene (TBLG, homo bilayer) and graphene–hBN moiré superlattices (hetero bilayer) using Raman spectroscopy supported by theory. In TBLG, the G mode exhibits a clear twist-angle evolution: it broadens, splits, and develops additional resonances in the small angle regime, consistent with moiré-modified phonon interactions. At larger twist angles, these features progressively collapse back into a single G peak response, indicating a diminished role of reconstruction. In graphene hBN moiré superlattices, we instead observe moiré-induced Raman modes appearing on both sides of the G peak, while the central G mode remains largely insensitive to twist angle. Our calculations associate the emergent modes with specific reconstructed stacking regions, establishing a direct link between twist angle, lattice reconstruction, moiré phonons, and interlayer coupling opening pathways for controlling phononic, optoelectronic, and thermal functionality in future van der Waals heterostructures.

References

[1] Sushil Sahu et al. Probing Phonon Modes in Reconstructed twisted Homo and Hetero Bilayer System (arXiv:2506.19669)

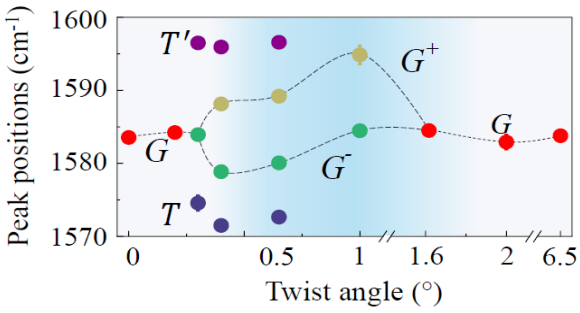

Figure1: Evolution of the positions of multiple resonant peaks near the G mode as a function of twist angle in twisted bilayer graphene (TBLG). A pronounced peak splitting appears at intermediate twist angles, where lattice reconstruction is strongest, while at larger twist angles the features progressively merge back toward a single peak.