Theoretical modeling of twist-angle-dependent plasmon resonances in moiré 2D materials

Shuva Mitra and Irena Knezevic
Department of Electrical and Computer Engineering
University of Wisconsin-Madison, Madison, WI 53706, USA
smitra8@wisc.edu, irena.knezevic@wisc.edu

Moiré superlattices, formed by stacking two-dimensional (2D) materials with a twist angle between them or stacking two lattice-mismatched materials, have recently emerged as versatile platforms for exploring novel quantum phenomena [1]. In addition to the usual control parameters such as doping, gating, straining, and external electromagnetic fields, the twist angle provides additional control as the electronic properties of the materials highly depend on the twist angle. Figure 1 shows the emergence of moiré patterns in two single-layer graphene with a twist angle. The introduction of twist angle in moiré systems modifies the interlayer coupling and gives rise to flat electronic bands and miniband formation.

Surface plasmon polaritons, hybrid excitations that bear signatures of both electromagnetic waves and collective electron waves and are formed at the surface of materials, are highly sensitive to the electronic band structure and dielectric environment and can be generated in various structures such as nanoribbons and nanomeshes [2], [3]. Twist-angle-dependent bandstructure of moiré structures provides an ideal platform for plasmon generation and control. Plasmons in 2D materials can control light beyond the diffraction limit with potential applications ranging in nanophotonics, biological sensing, photovoltaics, and nonlinear optics.

In this work, we investigate plasmons in twisted moiré superlattices. By employing theoretical models based on tight-binding and continuum approximations, coupled with numerical simulation using the density matrix formalism, we aim to explore how the twist angle, interlayer coupling strength, and dielectric environment control plasmon dispersion, lifetime, and confinement. Figure 2 shows the angle-dependent bandstructure of twisted bilayer graphene calculated via the tight-binding model in the continuum limit. Furthermore, the presence of localized flat bands in certain twist angles, such as the magic angles in twisted bilayer graphene, can enhance the electron–electron interactions, potentially leading to exotic plasmonic modes. We hypothesize that the interplay between moiré-induced minibands and long-range Coulomb interactions will lead to tunable plasmonic modes with wavelengths far below the diffraction limit, making them suitable for extreme light confinement. By achieving controllable plasmonic resonance over wide infrared frequency range, twisted bilayer materials have potential nonlinear optics applications such as frequency comb generation. Additionally, the quantum nature of these plasmons in moiré systems could pave the way for hybrid quantum systems where plasmonic excitations couple with quantum emitters or other quasiparticles, such as excitons and phonons.

In conclusion, we presented a numerical study of plasmons in twisted bilayer 2D materials. Tuning the band structure and bandgap with twist angle provides a platform for generating tunable plasmons. This microscopic simulation results can be effective in designing in next-generation 2D material-based plasmonic and nonlinear optoelectronic devices.

Acknowledgment

This work was funded by NSF Award No. 2212011 ECCS, Splinter Professorship, and Vilas Distinguished Achievement Professorship (IK). Calculations were performed at CHTC (UW-Madison).

References

[1] E. Y. Andrei and A. H. MacDonald, “Graphene bilayers with a twist,” *Nat. Mater.*, vol. 19, no. 12, pp. 1265–1275, Dec. 2020.
[2] F. Karimi and I. Knezevic, “Plasmons in graphene nanoribbons,” *Phys. Rev. B.*, vol. 96, no. 12, Sep. 2017.
[3] F. Karimi, S. Mitra, S. Soleimanikahnoj, and I. Knezevic, “Plasmon-enhanced optical nonlinearity in graphene nanomeshes,” *Phys. Rev. B.*, vol. 108, no. 3, Jul. 2023.

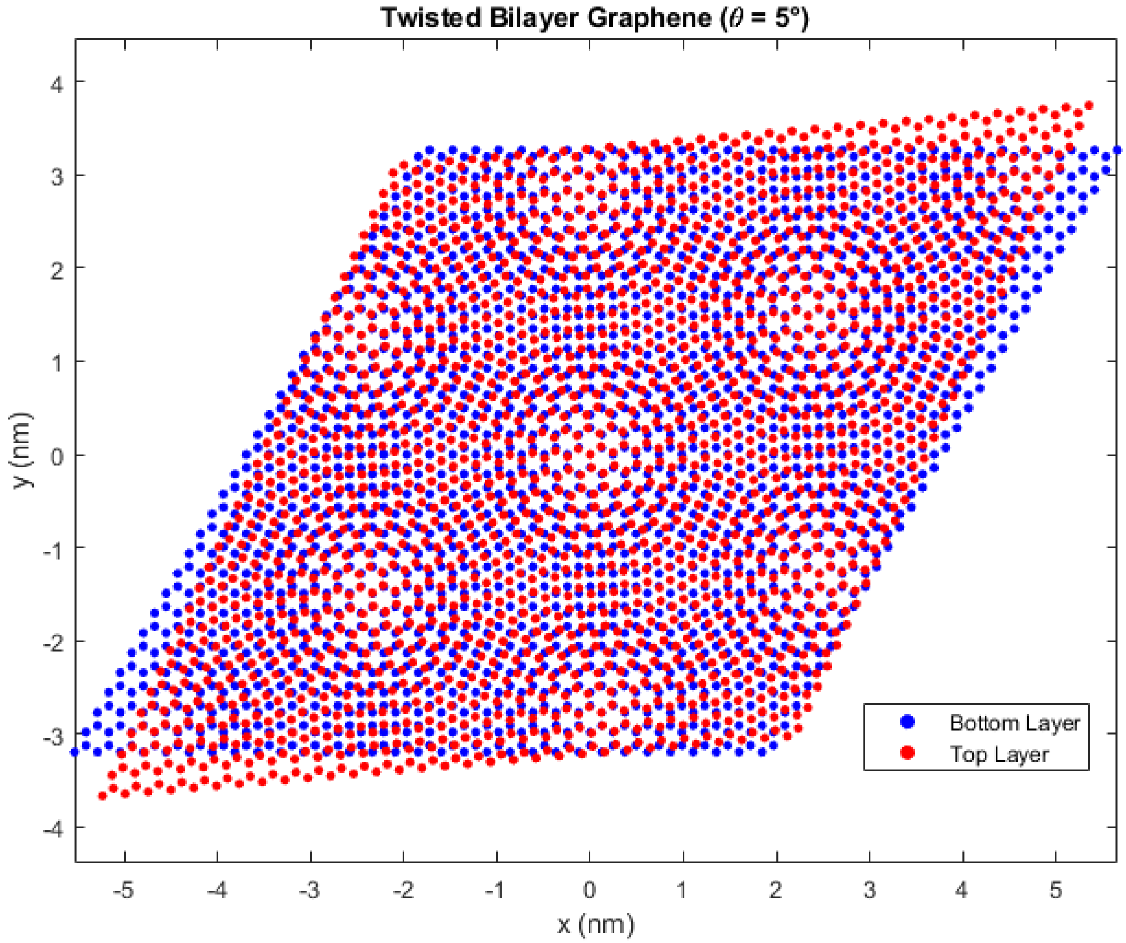
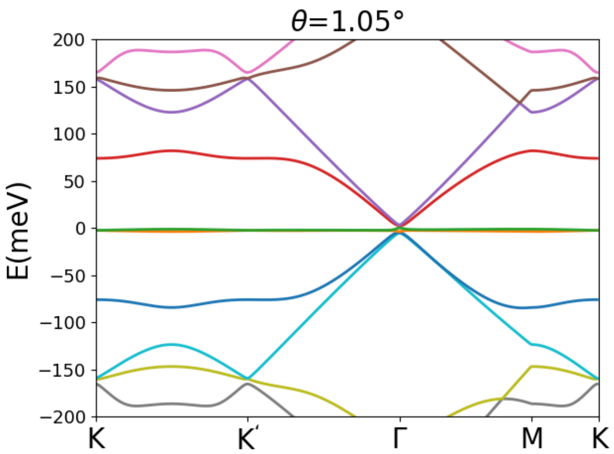
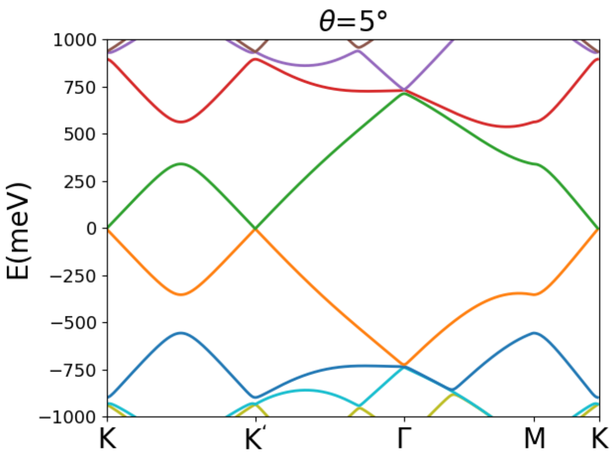


Fig. 1: Two graphene layers with a small twist angle between them creating a moiré pattern with large periodicity.



(a)



(b)

Fig. 2: Twist-angle-dependent tunable bandstructure in bilayer graphene. (a) Flatbands at magic twist angle and (b) single-layer-graphene-like linear bands.