Angle-resolved photoemission spectroscopy of graphene van der Waals heterostructures

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Angle-resolved photoemission spectroscopy (ARPES) is a powerful method of exploring the electronic band structure of solids, in particular 2D materials. Here, we study theoretically ARPES spectra of bi- and tri-layer stacks of graphene with one twisted interface.

We model ARPES spectra of twisted bilayer graphene for a broad range of the twist angle θ, from the "magic angle" limit of ~1° to the maximum twist angles of ~30° [1]. The momentum resolution of ARPES as well as sensitivity to chirality of electrons in graphene allows us to track the positions of the Dirac points across the "magic angle" condition of a flat miniband. At the same time, we show that for large angles, Bragg scattering on moiré superlattice leads to significant changes in the vicinity of the M points of the graphene Brillouin zone.

In contrast, stacks of three layers, with two forming a Bernal bilayer and the third one twisted are special because they are the thinnest structures that contain both aligned and misaligned configurations. While the former can be easily described using real-space tight-binding model, the latter is commonly modelled by coupling graphene electrons in the reciprocal space. The complementarity of the two spaces allows us to build a model in which the interatomic potential between carbons is described in a self-consistent fashion [2]. We show that ARPES spectra of twisted trilayer graphene allow determination of this potential for a simple ansatz without additional external input. Importantly, our approach can be applied to many other van der Waals interfaces.

Figures

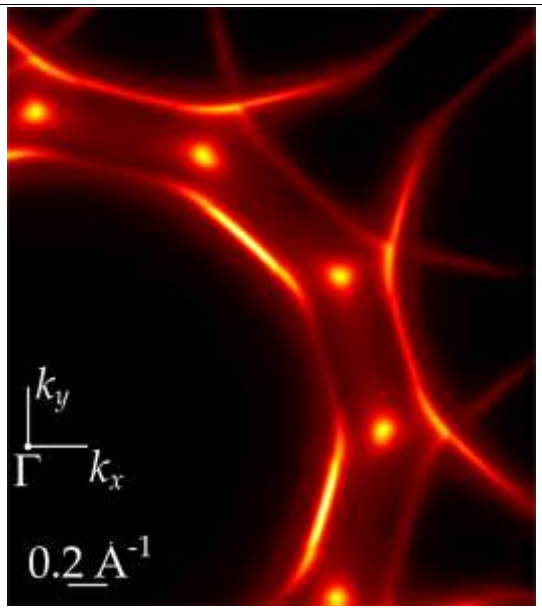

Figure 1: Simulation of ARPES constant-energy map of twisted bilayer graphene with twist angle of 28° at energy of 2.4 eV below the neutrality points.

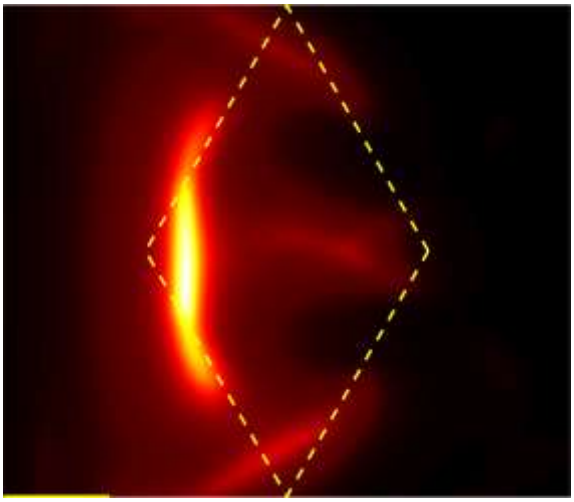

Figure 2: Simulation of ARPES constant-energy map of twisted bilayer graphene with twist angle of 5.2° at energy of 0.56 eV below the neutrality points. The yellow rhombus shows the boundaries of the superlattice Brillouin zone.

References

[1] A. Garcia-Ruiz Fuentes *et al.*, in preparation (2019).
[2] J. J. P. Thompson *et al.*, in preparation (2019).