Heterostrain physics of Twisted Bilayers of Graphene near magic angle

Florie Mesple
Guy T. de Laissardière [2], Ahmed Missaoui [2], Claude Chapelier [1], Vincent Renard [1]
[1] *Université Grenoble Alpes, CEA, IRIG, PHELIQS, 38000 Grenoble, France*
[2] *LPTM, Université de Cergy-Pontoise-CNRS, F-95302 Cergy-Pontoise Cedex, France*
florie.mesple@cea.fr

In twisted bilayers of graphene (TBLG) the moiré pattern induces electron correlated physics when the rotation between the layers is close to a so called magic angle [1]. Recent STM (Scanning Tunneling Microscopy) measurements have evidenced a doping dependent energy gap indicating a splitting of the flat band predicted for the magic angle system without correlations [2, 3, 4, 5]. This gap has therefore been attributed to the new electron correlated physics. Yet, previous research [6, 7, 8] has shown that the moiré and its electronic structure are not only controlled by the rotation between the layers but also by the relative strain between them (heterostrain). It is therefore important to investigate the effect of heterostrain near the magic angle because it could have a strong impact on the observed electronic properties. In this context we use the method introduced in Ref. [6] to analyse STM data recently published on TBLG near the magic angle. This allows us to determine the relative arrangement of the layers in detail and to produce a realistic unit cell suitable for tight-binding calculations. These local density of states (LDOS) calculations are in good agreement with the published data for large dopings - when electron correlations can be neglected. This indicates that heterostrain effect is responsible for a large part of the observed energy gap, correlated physics expressing on top of this starting point. In addition, our calculations show that electronic properties depend on the amplitude of heterostrain but also on other fine details in particular on the angle at which uniaxial heterostrain is applied (Figure 1).

References

[1] Y. Cao et al., Nature 556 (2018)
[2] A. Kerelski et al., Nature 572, 95-100 (2019)
[3] Y. Choi et al., Nature Physics (2019)
[4] Y. Jiang et al., Nature volume 573, 91–95 (2019)
[5] Y. Xie et al., Nature 572, 101 (2019)
[6] L. Huder et al., Phys. Rev. Lett. 120, 156405 (2018)
[7] H. Shi et al., ArXiv, 1905.04515v2 (2019)
[8] G. Yu et al., npj compumats, 5:122 (2019)

Figures

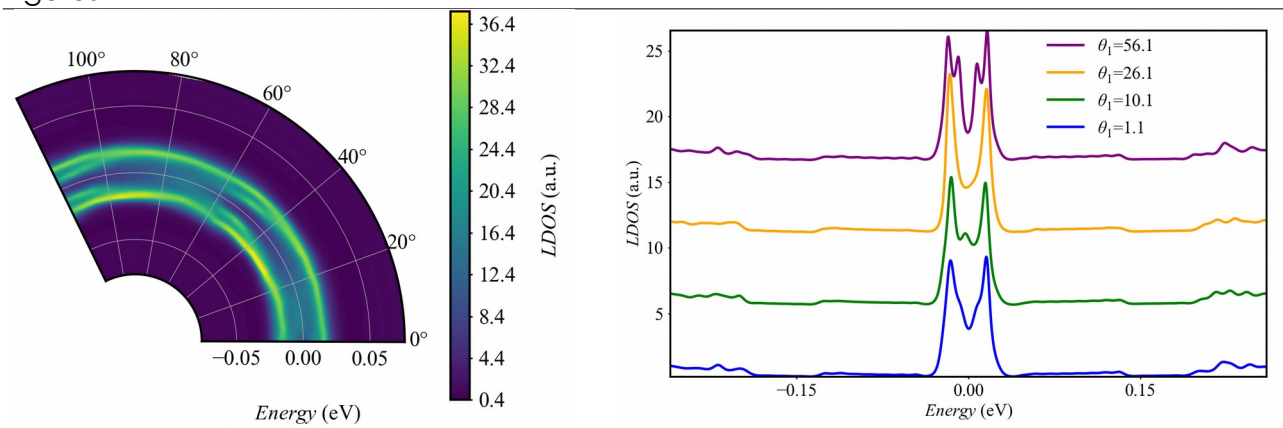

Figure 1: Tight-binding calculated LDOS of 1.10° TBLGs in AA zone, depending on the direction of application of a 0.4 % uniaxial strain : between 0° and 120° (**Left**) ; and for specific angles (**Right**).