Bruno Amorim

CeFEMA, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001, Lisboa, Portugal

bruno.a.c.amorim@tecnico.ulisboa.pt

General theoretical description of photoemission spectroscopy of van der Waals heterostructures

Abstract

Angle resolved photoemission spectroscopy (ARPES) is an extensively used tool to characterize the electronic properties of materials, generally interpreted as a direct probe to their electronic band structure. This view is not strictly true as the signal measured in ARPES is actually weighted by matrix elements, which describe the photo-induced electronic transition from a crystal bound state to a nearly free photoemitted electron state. These matrix elements can have a strong momentum dependence, which affect the visibility of different bands in ARPES. ARPES matrix elements are known to play an important role in cases where different bands are strongly coupled, such as in graphene and graphite [1], and in systems where there is a competition between different periodicities [2]. Both these effects are important in van der Waals (vdW) heterostructures - which are formed by stacked layers of different two-dimensional materials, with promising applications in electronics and light detection [3]. The lattice mismatch and/or misalignment between different layers naturally leads to a competition between periodicities. Therefore, in vdW structures ARPES cannot be interpreted as a direct probe to the electronic band structure. I present a general theory [4], based on tight-binding Hamiltonians, to model ARPES in both commensurate and incommensurate vdW heterostructures with arbitrary lattice mismatch/misalignment. As an example, I apply the general method to the case of twisted bilayer graphene, obtaining the ARPES bands and ARPES constant energy maps. The present theory should be useful in correctly interpreting experimental ARPES results of vdW structures and other system displaying competition between different periodicities, such as density wave phases.

References

[1]   E. L. Shirley et al., PRB 51 (1995) 13614
[2]   J. Voit et al., Science 290 (2000) 501
[3]   K. S. Novoselov and A. H. Castro Neto, Phys. Scr. 2012 (2012) 014006
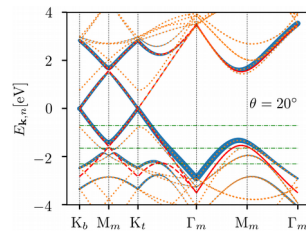[4]   B. Amorim, arXiv:1711.02499 (2017)

Figures

Figure 1: Computed ARPES bands (thick blue lines, the thickness is proportional to the visibility of the bands) and band structure (dotted yellow lines) for bilayer graphene with a twist angle of 20°. The ARPES bands mostly follow the bands of the decoupled layers (red dashed lines). The horizontal lines represent the energies at which the constant energy maps of Figure 2 are computed.
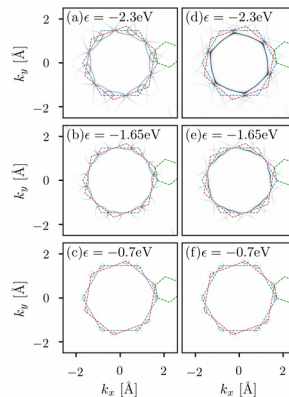

Figure 2: Computed ARPES constant energy maps for bilayer graphene with a twist angle of 20°. (a-c) ARPES maps in the absence of coupling between the layers. (d-f) Reconstructed maps due to interlayer coupling. The crescent shape of the constant energy surfaces is due to the ARPES matrix elements.