Twist angle dependence of the electronic structure in graphene antidot lattices with hBN encapsulation

Yongping Du[1,2]
Antti-Pekka Jauho[1,2]
[1]*Center for Nanostructured Graphene, Technical University of Denmark, Kongens Lyngby, Denmark*
[2]*DTU Physics, Technical University of Denmark, Kongens Lyngby, Denmark*
Email: antti@dtu.dk; yondu@dtu.dk

Abstract

Recent measurements confirm the theoretical prediction [1] that graphene antidot lattices may have a sizable band gap [2]. However, the dependence of the properties of the antidot lattice on the twist angle between the encapsulating hBN layers and the nanostructured graphene has not yet been the subject of a systematical experimental study. It is known that dramatic effects may occur for a graphene bilayer at certain twist angles, such as unconventional superconductivity or correlated insulator behavior [3,4] and it is a natural question to ask whether antidot lattices display intriguing behavior as the twist angle is varied. It has already been shown that the Moiré interaction between graphene and hBN can clone the Landau fan [2]. Here, we perform a theoretical investigation of antidot lattices in twisted heterostructures consisting of graphene and hexagonal boron nitride (G/hBN). By using first-principles calculations, we systematically investigate how the twist angle affects the electronic structure in these systems. Our numerical results (Figure 1) show that the band gap of a pristine G/hBN structure decreases monotonously as the twist angle is increased. However, for G/hBN with an antidot lattice, the band gap shows a complicated dependence on the twist angle. Theoretical studies as the ones described here are essential in the design of twistronic devices utilizing antidot lattices.

References

[1] T. G. Pedersen *et al.*, Phys. Rev. Lett. **100**, 136804 (2008).
[2] Bjarke S. Jessen, Lene Gammelgaard, Morten R. Thomsen *et al.* Nature nanotechnology, **14** (2019) 340-346.
[3] Yuan Cao, Valla Fatemi, Shiang Fang *et al.* Nature **556** (2018) 43-50.
[4] Yuan Cao, Valla Fatemi, Ahmet Demir *et al.* Nature **556** (2018) 80-84.

Figures

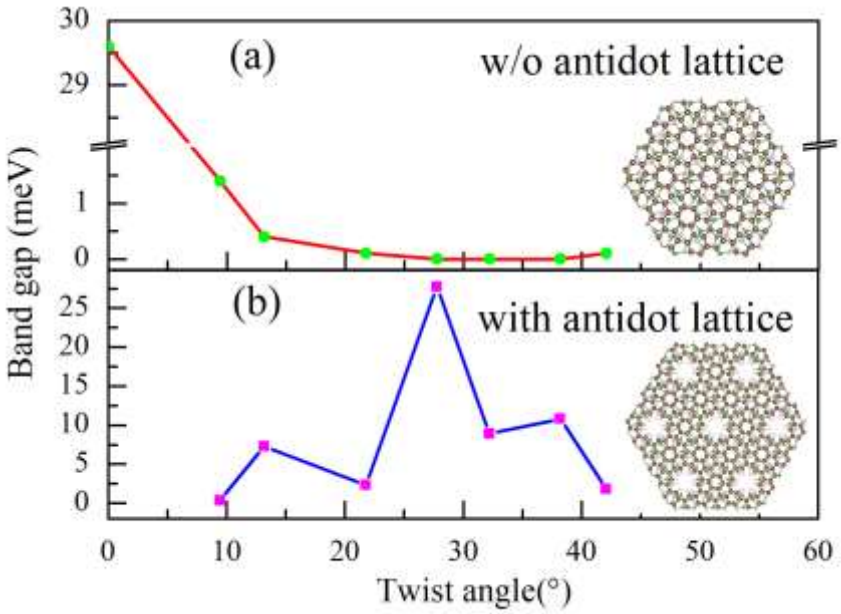

Figure 1: Calculated band gap of G/hBN bilayer as a function of twist angle. (a) Twisted bilayer without an antidot lattice - the band gap decreases as the twist angle increases; (b) Twisted bilayer with an antidot lattice (antidot diameter is 5.754Å) – maximal band gap is observed at twist angle ≈ 30 deg.