Highlights

Electronic and thermal transport from the nanoscale to the macroscale - 2018

Crucial role of atomic corrugation on the flat bands and energy gaps of twisted bilayer graphene at the magic angle θ ~ 1.08◦

Procolo Lucignano[1], Dario Alfè[2,3], Vittorio Cataudella[3,1], Domenico Ninno[3,1], and Giovanni Cantele[1]

[1]CNR-SPIN, c/o Complesso di Monte S. Angelo, via Cinthia, 80126 Napoli, Italy
[2]Department of Earth Sciences and London Centre for Nanotechnology, University College London, Gower Street, London WC1E 6BT, United Kingdom
[3]Dipartimento di Fisica "Ettore Pancini," Università degli Studi di Napoli "Federico II," Complesso di Monte S. Angelo, via Cinthia, 80126 Napoli, Italy

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Among the most recent approaches to device engineering, *twistronics* has received tremendous attention in the last two years. The basic concept is that of twisting the angle between layers composing two-dimensional van der Waals heterostructures, such as a graphene bilayer. Just two-years ago, some scientists discovered that at "special" twist angles, referred to as *magic angles*, the properties of a twisted bilayer graphene can dramatically change [Y. Cao, *et al.*, Nature 556, 80 (2018); Nature 556, 43(2018)]. At the first magic angle, θ~1.08°, a novel superconducting phase, reminiscent of that of that of the underdoped cuprates and with a critical temperature ranging from 1.7 to 3 K shows up. Moreover, a flat band (FB) manifold emerges close to the Dirac points, with a very tiny dispersion (experimentally estimated to be ~10 meV) and separated by energy gaps ~50 meV from both lower and higher energy bands. Such FBs are also responsible for an insulating phase observed by tuning the chemical potential through an external gate.

The nature, role and origin of such FBs is being debated in the literature, even though no common consensus has been reached yet. In this work we enlighten, from state-of-the-art, first principles calculations, the low-energy properties of twisted bilayer graphene. In particular, we unequivocally identify the atomic relaxation, following the twisting of the bilayer, as the main factor determining the emergence of the FBs close to the Fermi energy. If the atomic corrugation (see figure 2 for a relief map of the displacement) is not taken into account, the energy gaps separating the FBs from the lower and higher energy bands cannot be correctly predicted.

The work has been selected by the editors of Physical Review B to be an Editors' Suggestion.

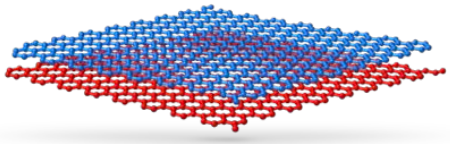

Fig. 1: A schematic view of twisted bilayer graphene.

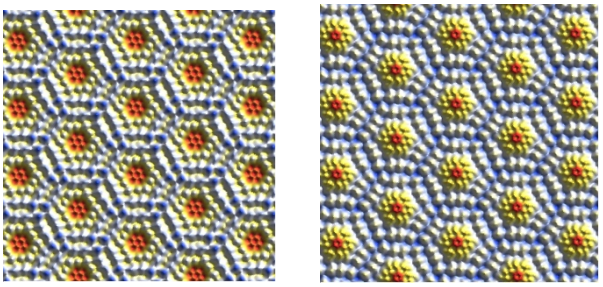

Fig. 2: A color map of the atomic relaxations in the bottom and top plane of twisted bilayer graphene at the first magic angle.