Pseudo magnetization in twisted bilayer graphene under hydrostatic pressure

Francisco Sanchez-Ochoa
Instituto de Física, Universidad Nacional Autónoma de México, Ciudad Universitaria, Mexico City, Mexico
fsanchez@fisica.unam.mx

Twisted Bi-Layer Graphene (TBLG) is a rich platform to study novel phenomena, such as unconventional superconductivity, Mott insulating states, orbital magnetism, and spin Hall effect among other interesting phenomena. Despite the great efforts to describe properly the electronic structure of this TBLG at low angles with thousands of atoms through tight-binding calculations or continuum models; these parametrized methodologies tend to overestimate the electronic bandwidths and energy gaps at low energies due to a bad description of relaxation effects in TBLG. Here using density functional theory (DFT) calculations with GGA (PBE) plus an optimized single basis set per orbital, we study several commensurate angles of TBLG under hydrostatic pressure. This is done to achieve flat bands at larger angles, see left panel of Figure 1, and indeed to demonstrate the appearance of pseudomagnetic (B) and potential (V) fields in these graphitic materials generated through in-plane strain by the external pressure, see right panel of Figure 1. We expect these results guide more future experimental and theoretical studies.

Figures

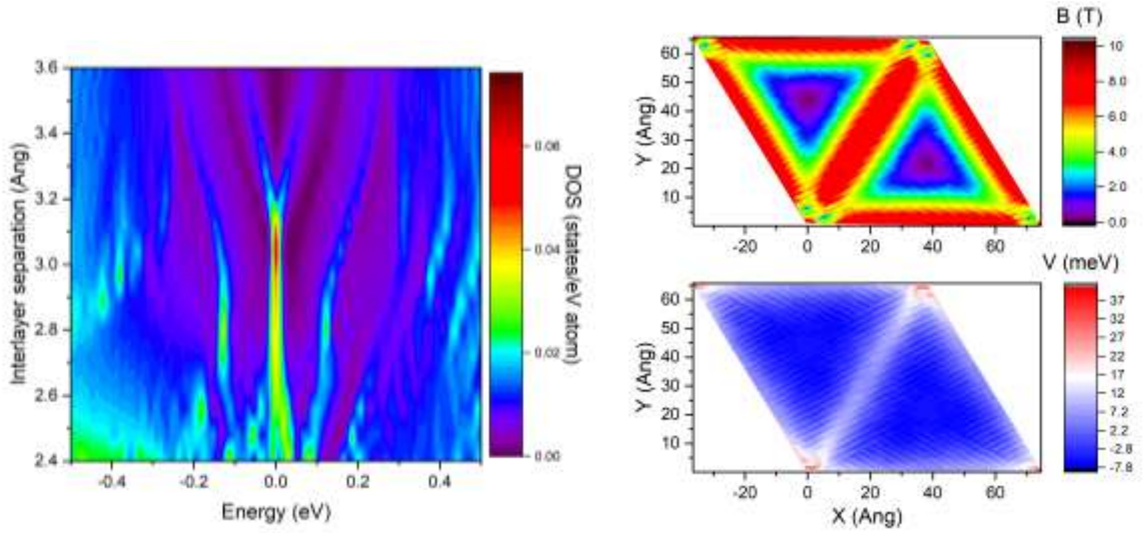

Figure 1: TBLG with θ=1.89° and 3676 atoms. Left panel: density of states (DOS) as a function of interlayer separation and energy. Right panel: Pseudomagnetic (B) and potential (V) fields for the upper graphene layer having an interlayer separation of 2.4 Ang.

Acknowledgements: This work was supported from CONACYT Mexico Grants No. A1-S-14407 and No. 1564464.