Electronic properties of stacking faults in Bernal graphite

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In spite of the last century of research into the physical properties of graphite, this material regularly displays new, unexpected features enabled by the variations of stacking between van der Waals coupled layers [1,2]. Here, we show that a stacking fault in bulk graphite hosts a band of two-dimensional electrons [3] clearly distinguishable from the bulk carriers. Using a self-consistent tight-binding model of graphite, incorporating all Slonczewski-Weiss-McClure parameters- [1,2], we compute the dispersion and quantum topological characteristics of the two-dimensional band, we calculate the Landau level spectrum in magnetic field and the related Shubnikov-de Haas oscillation parameters, as well as the cyclotron mass of the two-dimensional carriers. We also show that most of the features of the fault-bound states are inherited from another celebrated graphitic system, rhombohedral trilayer graphene, which represents the central structural block of the stacking fault. The computed frequency of Shubnikov-de Haas oscillations and the cyclotron mass of the fault-bound charge carriers (at the Fermi level) are sufficiently different from the corresponding bulk values in graphite, making such stacking faults identifiable by quantum transport and cyclotron resonance measurements.

References

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[3] D. P. Arovas and F. Guinea. Phys. Rev. B, 78:245416, Dec 2008.

Figures

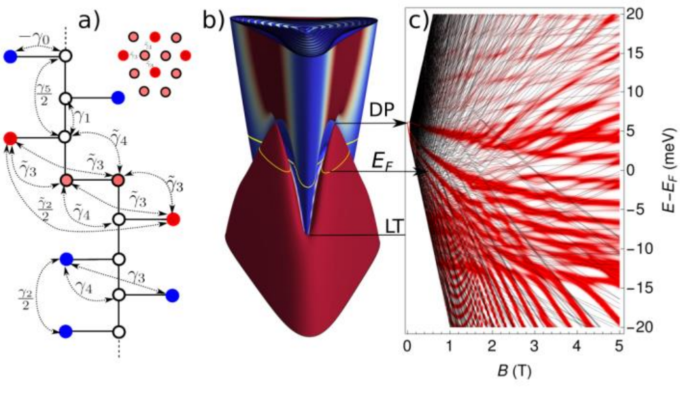

Figure 1: a) Schematic of the ABC stacking fault embedded in Bernal graphite, with labelled hopping parameters. b) Low-energy bands of a 30+1+30 layer system with red and blue colour indicating states localized on 3 ABC stacked layers of a stacking fault and the bulk graphite states respectively. The fault-bound 2D band features the Dirac points (DP) in three conic branches which merge together at energies below the Lifshitz transition (LT). c) Corresponding Landau levels (black thin lines) superimposed on a density of states projected onto 3 ABC stacked layers of a stacking fault (in red). Horizontal arrows indicate the states in the band structure which develop into their corresponding LLs in finite B field.