

# Computational Studies of Two-Dimensional Materials: From Graphene to Few-Layer Graphene and Beyond

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## Abstract

It has become possible in recent years to fabricate and manipulate two-dimensional (2D) nanomaterials in the laboratory that are as thin as one to few atomic layers. A well-known example is graphene, where the Dirac-Weyl Hamiltonian for massless fermions describes the low-energy quasiparticles. Intriguing physics has been found in these few-layer systems, and phenomena originally associated with particle physics can now be observed in condensed matter systems. In this talk, I will focus on our recent theoretical and computational studies of a few representative systems. These two-dimensional atomic layer systems provide a unique platform to probe the rich physics involving multiple interacting massless fermions.

It has been found that graphene layers grown epitaxially on SiC or by the chemical vapor deposition method on metal substrates display a stacking pattern with adjacent layers rotated by an angle with respect to each other. Our calculation shows that anisotropic transport properties manifest in a specific energy window, which is accessible experimentally in twisted bilayer graphene. The quasiparticle states in two distinct graphene layers act as neutrinos with two flavors, and the interlayer interaction between them induces an appreciable coupling between these two “flavors” of massless fermions, leading to neutrino-like oscillations [1].

The energy spectrum under an external magnetic field in twisted bilayer graphene also exhibits intriguing properties. The Hofstadter butterfly spectrum for Landau levels in a two-dimensional periodic lattice is a rare example exhibiting fractal properties in a truly quantum system. However, the observation of this physical phenomenon in a conventional material will require magnetic field strengths several orders of magnitude larger than what can be produced in a modern laboratory. It turns out that for a specific range of rotational angles twisted bilayer graphene serves as a special system with a fractal energy spectrum under laboratory accessible magnetic field strengths. This unique feature arises from an intriguing electronic structure induced by the interlayer coupling. Using a recursive tight-binding method we systematically map out the spectra of these Landau levels as a function of the rotational angle [2]. Our results give a complete description of LLs in twisted bilayer graphene for both commensurate and incommensurate rotational angles and provide quantitative predictions of magnetic field strengths for observing the fractal spectra in these graphene systems.

In addition, it has been shown recently that silicene, a 2D graphene-like form of silicon, may be synthesized epitaxially on the surface of a silver substrate [3] or on diboride thin films grown on silicon wafers [4]. This suggests new perspectives for the applications of massless fermions in materials that are compatible with Si-based electronics. Silicene has a buckled honeycomb arrangement of Si atoms with an electronic dispersion resembling that of graphene. It is expected that many of the unique electronic properties of graphene can also be realized in this new 2D system. Most likely the samples will be synthesized on some forms of substrates, and the possibilities are abundant. We have performed first-principles calculations of silicene on graphene in order to understand the effect of substrate interaction on the physical properties of these systems [5]. The phonon properties and electron-phonon interaction of freestanding silicene [6] will also be discussed.

## References

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### Figures

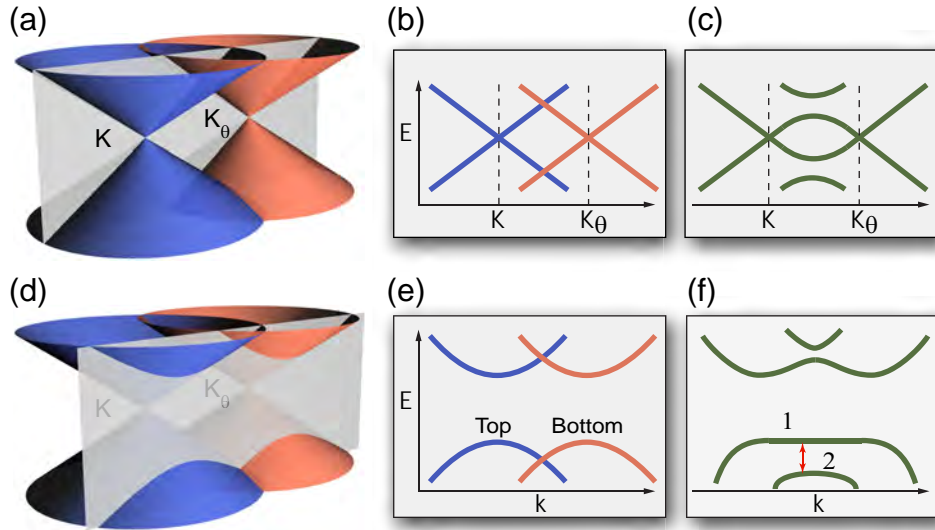


Figure 1. Schematic illustration of interlayer interaction in twisted bilayer graphene. (a) A plane cutting through the Dirac points of the two Dirac cones associated with the two twisted layers. The energy bands on the cross section shown in (a) are drawn in (b) and (c) for cases without and with interlayer interaction, respectively. (d) A plane cutting through the two Dirac cones without including the two Dirac points. The energy bands on the cross section shown in (d) are drawn in (e) and (f) for cases without and with interlayer interaction, respectively.

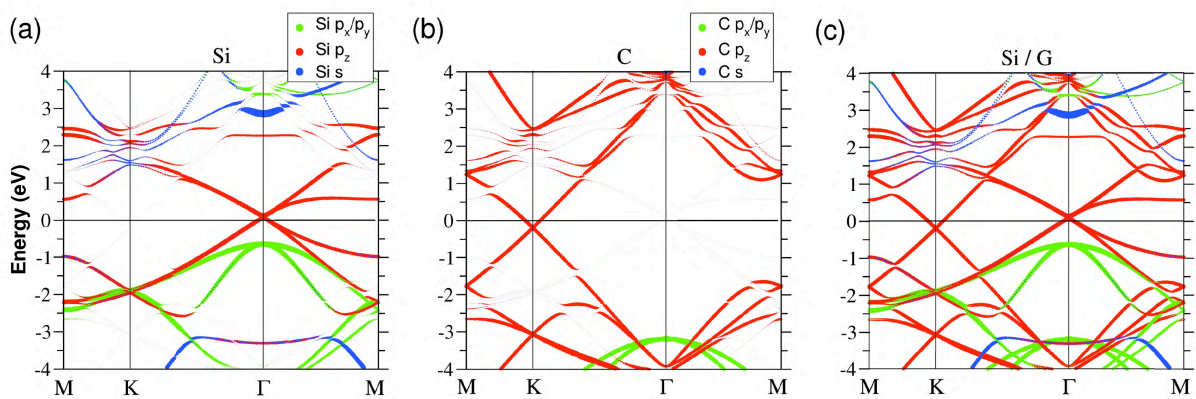


Figure 2. Band structure of Si(√3)/G(√7): (a) the projected states on Si are highlighted; (b) the projected states on C are highlighted; and (c) the projected bands in (a) and (b) are combined. The substrate-induced gap is about 26 meV for Si (Γ) and 2 meV for graphene (K), respectively.