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

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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 computational studies of a few representative systems, including the neutrino-like oscillation and anisotropic transport [1] in twisted bilayer graphene that also exhibits a rare fractal-like "butterfly" energy spectrum under external magnetic field [2]. In addition, I will also discuss the possibility of growing 2D structures of other group-IV elements on graphene. It is expected that many of the unique electronic properties of graphene can also be realized in this new 2D system. We have performed first-principles calculations of silicene on graphene [3] in order to understand the effect of substrate interaction on the physical properties of these systems. The phonon properties and electron-phonon interaction of freestanding silicene [4] will also be discussed.

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References:

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