Twistronics: the unconventional behavior of electrons in two-dimensional materials with a twist

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In the past few years, the field of twisted multilayer graphene and other two-dimensional layered materials, including families of insulators and semiconductors, has blossomed to the point of being referred with by a new term, “twistronics”. New structures, including multi-layers of successively twisted single layers, mixed layers, and multilayers of multilayers, are being studied experimentally and revealing ever richer behavior. We discuss theoretical investigations of some representative systems, starting with the iconic twisted bilayer graphene near the so-called magic angle, which produces a diverging (van-Hove singularity) density of states very close to the Fermi level of the neutral system (see Fig. 1). Our work is based on first-principles calculations which afford a full and accurate relaxation of atomistic degrees of freedom (see Fig. 2), which is essential in obtaining realistic single-particle states. These single-particle states can be used to derive effective hamitlonian models to describe the emergent phenomena of insulating and superconducting phases. We discuss how a realistic representation of localized single-particle states can be derived and how those can be employed in studying many-body physics related to Mott insulator behavior, superconductivity and other manifestations of correlated electronic states.