Electronic Properties of Twisted van der Waals Materials

By

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Abstract

Van der Waals materials are materials with strong in-plane covalent bonding and weak interlayer interactions. Due to the two-dimensional nature of these materials and interfaces naturally play a vital role in modifying their properties. This paper explores the electronic properties of twisted van der Waals structures and its promises. It also explores its applications and some key challenges facing 2D vdW layered materials.

I. Background

Van der Waals materials are materials with strong in-plane covalent bonding and weak interlayer (van der Waals) interactions and given the two-dimensional nature of these materials and interfaces naturally play a vital role in controlling or modifying their properties. The electronic properties of van der Waals structures can be significantly modified by the moiré superlattice potential, which strongly depends on the twist angle among the compounds [1]. Moreover, controlling the twist angle between layers is essential in tuning the interlayer coupling. The functionality of these heterostructures is also determined by the alignment of electronic energy bands between consecutive layers [2].

Since the discovery of graphene, efforts of researchers on two-dimensional van der Waals (vdW) materials has increased, with bilayer graphene considered as an ideal model system. Other materials include transition metal dichaclogenides (TMDs), hex-BN, and, heterostructures of single-layer GaS and GaSe [3]. According to both measurements and theoretical calculations [4] the interlayer vdW interactions and band structures of bilayer graphene can be greatly modulated by the twist angle between two neighboring graphene layers.

Furthermore, the two graphene layers are frequently electronically decoupled and each layer behaves as a monolayer graphene for large twist angles of > 5.5° except for a small set of angles that provide comparable structures [5,6]. Low-energy Van Hove singularities (VHSs) of twisted bilayer graphene (TBG) gradually moves closer as the twist angle decreases, accompanied by a significant suppression of Fermi velocity due to the strong interlayer coupling [7,8]. The Fermi velocity almost vanishes when the twist angle approaches the magic angle (~ 1.1°), leading to two highly non-dispersive flat moiré bands closely flanking the charge neutrality point. However, near the magic angle, an exceptionally wide range of correlated physics are observed experimentally in the TBG such as Mott insulator, superconductivity, ferromagnetism, and topology [9,10].

These two-dimensional materials (2D) with their heterostructure interface manipulating bring infinite possibilities and many unprecedented devices in electronics. These include electronic nanodevices, spintronics for low-power electronics, efficient spin transport, spin relaxation, and spin logic devices based on graphene and transition metal dichalcogenides (TMDs) [11]. Also, due to large mobile carriers of monolayer TMDs, it used for 2D-channel TFETS which combines the advantages of an atomically thin 2D channel with the high sensitivity of a TFET and can also be adapted into a revolutionary new class of biosensors [12].

II. Perspective; Challenges and Promises

Some key challenges facing 2D vdW layered materials are ohmic contact, carrier multiplication, valleytronics, Weyl semimetals, heterointerface, doping, and growth issues of heterostructures. 2D semiconductors find it difficult to form high-quality electrical contacts due to the layered nature that gives rise to van der Waals bonds to other 2D and 3D materials. However, recent theoretical and experimental advances on the nature of charge transfer across a 2D material interface (so-called seamless electrical contacts) have helped in the development of low-resistance contacts [13,14]. Also, the extremely long spin lifetime of carrier in graphene makes it suitable for a spin transport layer. The graphene and MCh2 semiconductor heterostructures demonstrate a high efficiency of spin injection from MCh2 to graphene. This brings up the possibilities of using 2D heterostructures for spintronic devices [15].

Furthermore, controlling the carrier type as well as concentration is a crucial issue in the semiconductor industry. Also, dopants can generate unpredicted physical properties for the host materials. However, the effort to create magnetic carrier by doping semiconductors with magnetic atoms, known as dilute magnetic semiconductors offers possibilities for solving this issue [16]. In addition, the nature of 2D magnetic properties allows for more opportunities for coupling the magnetic with electric field effects. Although a few examples of direct growth of heterostructures have been demonstrated, difficulties arise from the choice of initial substrate, in particular when the vertical heterostacking is considered. Graphene and h-BN layers offer great possibility owing to their thermal stability. TMDs can also be used as a substrate although the relative thermal stability should be taken into account in comparison with the host material [17].

Ultimately, the electronic properties of 2D vdW layered materials are certainly interesting from scientific and technological points of views and have been intensively investigated for a decade or so. There are still numerous challenges to be overcome as well as opportunities to be explored.

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