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First principles studies on electronic and transport properties of edge contact graphene-MoS_2 heterostructure

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ABSTRACT

Nanodevice based on MoS_2 channel lateral connecting with graphene electrode was fabricated in recent experiment. In present paper, first principles calculations are carried out to reveal the relationship between contact geometries and electrical properties of graphene-MoS_2 heterostructure. Four different contact edges between graphene and MoS_2, namely, Armchair-Armchair, Zigzag-Armchair, Armchair-Zigzag, Zigzag-Zigzag, are investigated. Calculations indicate that MoS_2 will be metalized as a consequence of junction formation with graphene. The metallic states located at Fermi level are mainly laid at the contact interface and dominated by 4d states of Mo atom as well as 2p states of both S and C atoms. Different contact geometries of graphene-MoS_2 result in different charge transfer values in contact interfaces. Investigation on band alignments reveals that n-type Schottky contacts are formed in four graphene-MoS_2 lateral heterostructures with barrier heights of 0.45–0.75 eV, which are larger than those of edge contact with Sc and Ti metals. The transmission gap of each configuration obtained using a two-probe system is unexpectedly larger than the intrinsic band gap of MoS_2. The discrepancies of current-voltage behavior in two represented configurations demonstrate that contact geometries play an important role in electronic transport properties of graphene-MoS_2 junctions.

1. Introduction

Since the discovery of graphene, two-dimensional (2D) materials have attracted enormous experimental and theoretical interests [1–4]. Among them, the semiconductor transition metal dichalcogenides (SCTMDs), such as MoS_2, WS_2, are promising materials due to their distinctive electronic and optical properties [5–10]. Unlike zero band gap nature of graphene, the occurrence of moderate band gaps makes them potential candidates for nanodevice applications. Field-effect transistors (FETs) based on MoS_2 exhibit large on/off ratios and near theoretical subthreshold swing values [5,11,12]. However, further improvement of the devices performance have been limited by relatively low carrier mobility, which mainly arise from the contact with metal electrode generating large contact resistance owing to the formation of Schottky barrier [13–16]. Therefore, great efforts have been made to optimize electrode contacts with MoS_2 [17–20].

Top contact and edge contact are two fundamental interface geometries between electrodes and 2D materials. Conventional methods usually use 3D metal electrodes to top contact with 2D MoS_2. Ohmic contacts can be achieved by choosing metals with suitable work functions for MoS_2. Nevertheless, it is difficult to obtain stable and controllable Ohmic contact in experiments. For example, Ohmic and Schottky contacts were found in the MoS_2 transistors with Au electrodes by different groups, respectively [5–21]. Theoretical studies have verified that edge contacts between 3D metal electrodes and 2D MoS_2 show more advantageous features compared with top contacts, owing to stronger orbital overlaps and better reduction of tunnel barriers [22]. Apart from 3D metal electrodes, 2D metallic TMDs and graphene, which can provide much smaller volumes, are also fabricated as electrode contacted with MoS_2. Graphene top contacts perform low contact resistances when they have sufficiently large contact areas [23,24], however, due to the van der Waals gap between graphene and MoS_2 [25], the contact resistance increases dramatically as the length of the graphene top contact is reduced below the transfer length to the tens of nm scale [26]. The metallic TMDs electrode forming edge contact with SCTMD can also generate smaller resistance [27,28], however, the metallic TMDs phase is metastable and this is not beneficial for its practical applications.

In recent experiments, the new lateral heterostructures, graphene-MoS_2 [26], are synthesized in spite of that the two atomic layers show significant crystallographic dissimilarity and

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possess large lattice mismatch (~25%). Moreover, the MoS_2-based devices in-plane stitched with graphene electrodes are also fabricated [29]. New graphene edge contact devices show low contact resistance, ohmic behavior at room temperature and the least possible additional volume to the devices. 1D edge contact exhibits significant potential for MoS_2 based future device applications. However, there is still a lack of knowledge of the precise edge morphology of the two materials stitched together, which may have great impact on the electronic and transport properties of the new in-plane heterostructure. Therefore, it is necessary to explore the relationship between the contact geometries and electrical properties of the heterostructure, which may contribute to practical device applications.

In this paper, we report a first-principle study on electronic and transport properties of edge contact between graphene and MoS_2. We construct four different edge contact configurations of

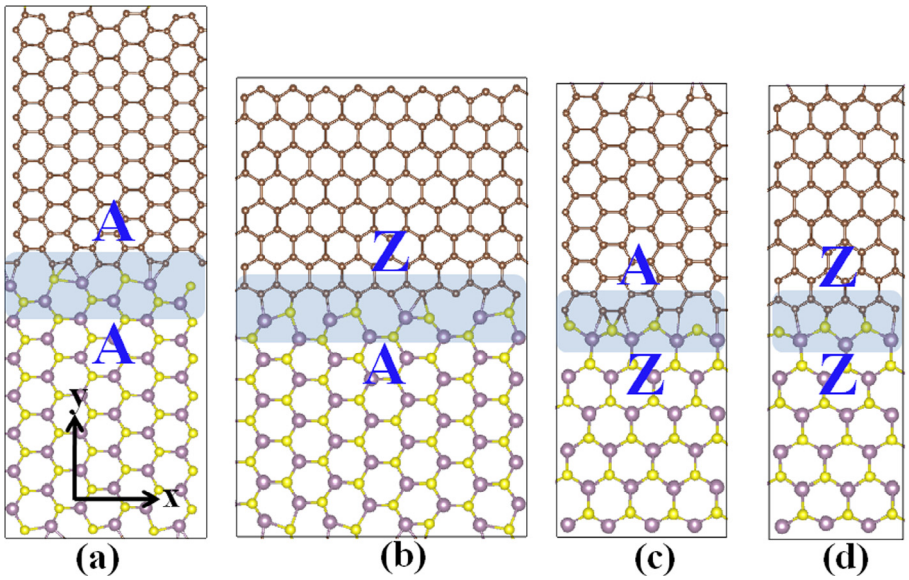

Fig. 1. Four edge contact geometries of graphene-MoS_2 heterostructures, (a) armchair-armchair, (b) zigzag-armchair, (c) armchair-zigzag, and (d) zigzag-zigzag. Shaded parts show the contact regions.

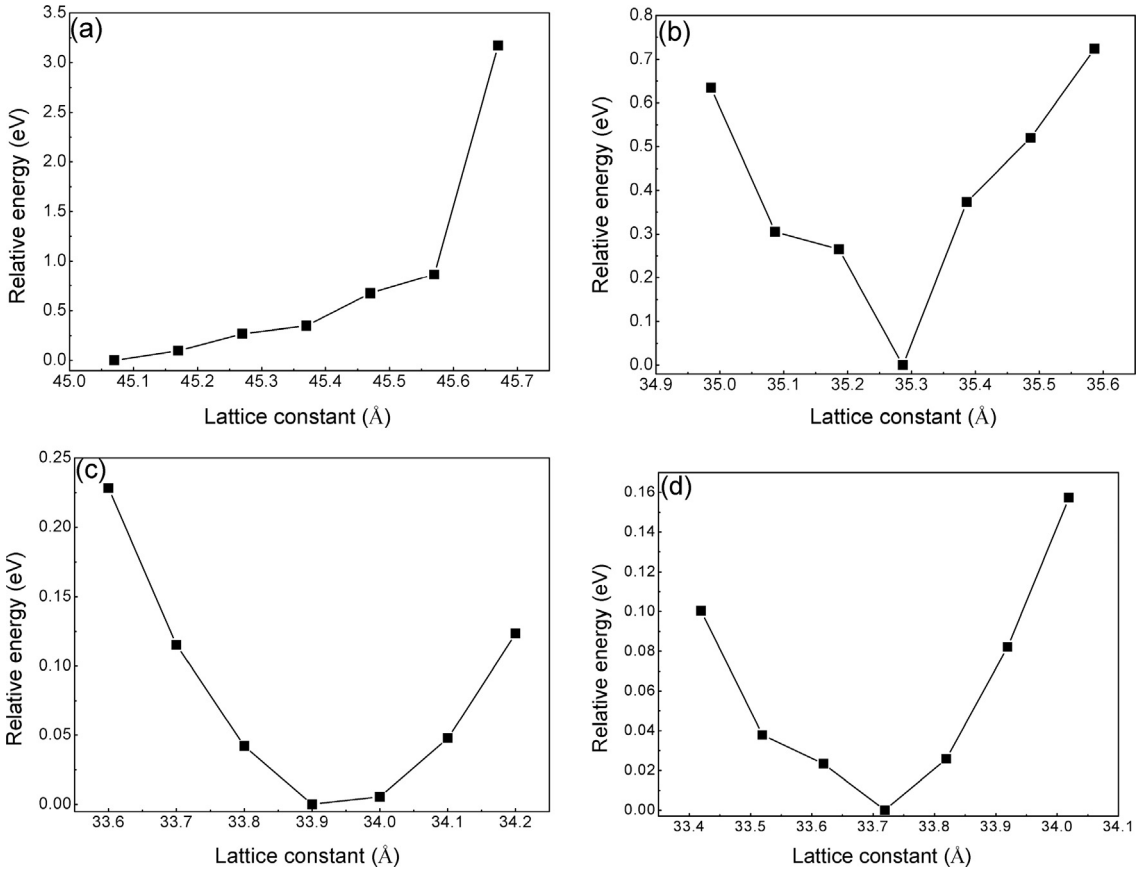

Fig. 2. The relative energy of (a) A-A, (b) Z-A, (c) A-Z, and (d) Z-Z junctions with different lattice constant along the direction vertical to the contact edge. The energy of the most stable configuration has been set to zero.