Electronic and transport properties of metal interface with monolayer 2H-MoS_2

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Abstract

Owing to their excellent properties, two dimensional materials along with metal contacts have attracted much towards device applications such as field effect transistors (FETs), photovoltaic devices, sensors and many more. With such a motivation, the present work explore in the direction of the electronic properties for metal contact with monolayer MoS_2 by using density functional theory simulations. We present the electronic properties for metal contact (Indium, gold and palladium) with 2D-MoS_2. The obtained electronic properties indicate n-type nature for metal depositions in the case of top contact. Furthermore, we find that gold contact is better in the view of orbital overlap, but Indium is favourable in terms of less Schottky barrier height. On the other hand, edge contact model results as strongly hybridized orbital overlaps and no Schottky barriers, which gives rise to the advantageous of edge contact interface as compared with top contact. We also examined the variation of Schottky barrier height with different metal atom work functions for both edge and top contacts. Going beyond standard electronic properties, we also perform the quantum transport simulations using nonequilibrium Greeen's function method to understand the contact nature at interface. From our simulations we find that indium provides another alternative deposition metal/electrode to obtain the Ohmic contact nature at the junction model.

Figure

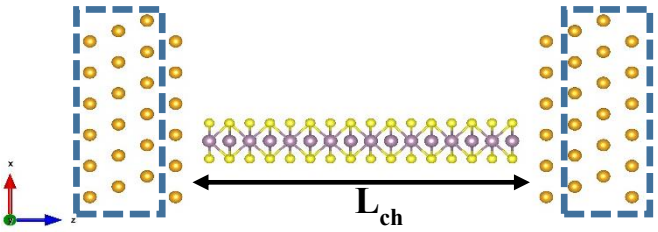

Figure 1: Snap shot of edge contact between metal atom and MoS_2