Effect of interfaces on electron transport properties of MoS$_2$ - Au Contacts

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Single layer MoS$_2$ is a promising material for future electronic devices such as transistors since it has good transport characteristics with mobility greater than 200 cm$^{-1}$ V$^{-1}$ S$^{-1}$ (comparable to the mobility achieved in thin silicon films or graphene nanoribbons) and on-off current ratios up to $10^8$ [1]. However, before MoS$_2$ can become a mainstream electronic material for the semiconductor industry, the design of low resistive metal-semiconductor junctions as contacts of the electronic devices needs to be addressed and studied systematically. We have examined the effect of Au contacts on the electronic transport properties of single layer MoS$_2$ by using density functional theory in combination with the non-equilibrium Greens function method. Charge density analysis shows the charge transfer from MoS$_2$ to Au contacts. The Schottky barrier between Au contact and MoS$_2$, transmission spectra, and I-V curves will be reported and discussed as a function of MoS$_2$ and Au interfaces of varying geometry. We will discuss our results in the light of recent experimental findings.