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Effect of interfaces on electron transport properties of MoS2–Au Contacts[1] MARAL AMINPOUR, University of Central Florida, Department of Physics, Orlando FL 32816-2385, USA, PROKOP HAPALA, Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnicka 10, 162 53, Prague, Czech Republic, DUY LE, University of Central Florida, Department of Physics, Orlando FL 32816-2385, USA, PAVEL JELINEK, Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnicka 10, 162 53, Prague, Czech Republic, TALAT S. RAHMAN, University of Central Florida, Department of Physics, Orlando FL 32816-2385, USA, RAHMAN'S GROUP COLLABORATION, NANOSURF LAB COLLABORATION — 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 $cm^{-1}V^{-1}s^{-1}$ 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 using density functional theory in combination with the non-equilibrium Green's function method. 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.

[1] B. Radisavljevic et al., Nature Nanotechnology **6**, 147 - 150 (2011).

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