Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Tuning the Schottky barrier heights at MoS_2|metal contacts: a first-principles study MOJTABA FARMANBAR , GEERT BROCKS, MESA+ Institute for Nanotechnology, University of Twente, The Netherlands — The nature of the Schottky barrier at metal contacts with the two-dimensional semiconductor MoS_2 is controversial. Using first-principles DFT calculations we show that the Schottky barrier height (SBH) for high work function (> 4.7 eV) metals typically obeys the Schottky-Mott limit, provided that a potential step that arises at the metal-MoS_2 interface is taken into account. It suggests that selecting a metal with an appropriate work function may reduce the SBH to zero. However, we find that for low work function metals the Fermi level is pinned below the conduction band edge of MoS_2 , leading to SBHs of 0.1-0.3 eV. We attribute the pinning to the metal-MoS_2 interaction at the interface perturbing the electronic structure of MoS_2 , and causing a broadening of the MoS2 conduction band edge. Inserting a monolayer of boron nitride (BN) between the metal surface and the MoS_2 layer disrupts this interaction. In addition the BN layer effectively decreases the metal work function, thereby enabling a line-up of the Fermi level with the MoS_2 conduction band with a vanishing SBH.

Mojtaba Farmanbar Gelepordsari
Twente Tech Univ

Date submitted: 14 Nov 2014 Electronic form version 1.4