Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Computational design of p-type contacts for MoS_2-based electronic devices PRIYANK KUMAR, Massachusetts Institute of Technology, TIZIANA MUSSO, ADAM FOSTER, Aalto University, JEFFREY GROSSMAN, Massachusetts Institute of Technology — The excellent physical and semiconducting properties of transition metal dichalcogenide (TMDC) monolayers make them promising materials for many applications. A well-known example is MoS_2, which has gained significant attention as a channel material for next-generation transistors. While n-type MoS_2 field-effect transistors (n-FETs) can be fabricated with relative ease, fabrication of p-FETs remains a challenge as the Fermi-level of elemental metals used as contacts are pinned close to the conduction band, leading to large p-type Schottky barrier heights (SBHs). Using *ab initio* computations, we design and propose efficient hole contacts utilizing high work function oxide-based hole injection materials, with the aim of advancing p-type MoS_2 device technology. Our calculations will highlight the possibility to tune and lower the p-type SBH at the metal/semiconductor interface by controlling the structural properties of oxide materials. Taken together, our results provide an interesting platform for experimental design of next-generation MoS_2-based electronic and optoelectronic devices.

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Date submitted: 13 Nov 2014 Electronic form version 1.4