Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Structural phase transitions in monolayer molybdenum dichalcogenides[1] DUK-HYUN CHOE, HA JUNE SUNG, KEE JOO CHANG, Deparment of Physics, KAIST — The recent discovery of two-dimensional materials such as graphene and transition metal dichalcogenides (TMDs) has provided opportunities to develop ultimate thin channel devices. In contrast to graphene, the existence of moderate band gap and strong spin-orbit coupling gives rise to exotic electronic properties which vary with layer thickness, lattice structure, and symmetry. TMDs commonly appear in two structures with distinct symmetries, trigonal prismatic 2H and octahedral 1T phases which are semiconducting and metallic, respectively. In this work, we investigate the structural and electronic properties of monolayer molybdenum dichalcogenides (MoX2, where X = S, Se, Te) through first-principles density functional calculations. We find a tendency that the semiconducting 2H phase is more stable than the metallic 1T phase. We show that a spontaneous symmetry breaking of 1T phase leads to various distorted octahedral (1T') phases, thus inducing a metal-to-semiconductor transition. We discuss the effects of carrier doping on the structural stability and the modification of the electronic structure.

[1]This work was supported by the National Research Foundation of Korea (NRF) under Grant No. NRF-2005-0093845 and Samsung Science and Technology Foundation under Grant No. SSTFBA1401- 08.

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Date submitted: 12 Nov 2014 Electronic form version 1.4