Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

First-principles study on native defects and dopant impurities in single-layer MoS2 JI-YOUNG NOH, Sookmyung Women's University, MINKYU PARK, KRISS-University of Science & Technology, HANCHUL KIM, Sookmyung Women's University, YONG-SUNG KIM, KRISS-University of Science & Technology — We have carried out first-principles calculations on the atomic and electronic properties of a single layer MoS2 with various native defects and substitutional dopants (V, Nb, Ta, N, P, As, Sb for n-type and Mn, Tc, Re, F, Cl, Br for p-type). For charged defects, various supercell sizes are considered to investigate the finite-size supercell effects, and we apply the electrostatic energy correction and level alignment to obtain the formation energies and transition levels of the isolated defects. We find that the S-vacancy and S-interstitial on top of a S atom have low formation energies among the native defects. The S-interstitial is found to be a neutral defect, while the S-vacancy is a deep acceptor. We discuss possible origins of the natural n-type doping in exfoliated single-layer MoS2 based on the substitutional dopant impurities.

Yong-Sung Kim
KRISS-University of Science & Technology

Date submitted: 15 Nov 2013 Electronic form version 1.4