Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Stability of $MoS_{2(1-x)}Se_{2x}$ alloy: insight from first-principles calculations[1] DUY LE, TALAT S. RAHMAN, Department of Physics, University of Central Florida — Two-dimensional transition metal dichalcogenide (TMD) alloy is an interesting class of TMD because the ability to tune continuously its bandgap opens many new possibilities for basic studies, device concepts, and fabrication of novel heterostructures. We will present phonon dispersions of $MoS_{2(1-x)}Se_{2x}$ alloy calculated using Density Functional Perturbation Theory (DFPT). The dispersions do not show any existence of instability modes for various Se concentrations (x), attesting the stability of this TMD alloy. We will, in addition, show electronic and optical properties, including Raman spectra, of $MoS_{2(1-x)}Se_{2x}$ alloy as a function of Se concentrations and their comparison with available experimental data.

[1]This work is supported in part by the US Department of Energy under grant DE-FG02-07ER15842.

Duy Le
Univ of Central Florida

Date submitted: 15 Nov 2013 Electronic form version 1.4