Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Strong coupling charge-density waves in doped transition metal dichalcogenides JUN-HO LEE, YOUNG-WOO SON, Korea Inst for Advanced Study — We present a theoretical study on a phase transition from quantum spin Hall insulating phase to strong coupling charge density wave (CDW) in adatom-doped single layer transition metal dichalcogenides (TMDs) $1T' - MTe_2$ (M = Mo and W) using first-principles calculation methods. It is shown that when $1T'$ phase TMDs are doped by alkali metals or hydrogen atom, their Fermi surface shows quasi-one-dimensional features and phonon dispersion at the corresponding nesting vectors becomes unstable, turning $1T'$ structure to diamond-shape (DS) chain phase with a substantial energy gap. The resulting CDW phase is compatible with a ground state of ReS_2 and $ReSe_2$. To unveil the origin of CDW phase transition, we calculate the electronic non-interacting susceptibility and electron-phonon coupling strength as a function of doping concentration and then find out that origin of phase transition is the strong electron-phonon coupling of the doped TMDs.

Jun-Ho Lee
Korea Inst for Advanced Study

Date submitted: 11 Nov 2016 Electronic form version 1.4