Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Topological phase transition in layered transition metal dichalcogenides DUK-HYUN CHOE, HA-JUN SUNG, KEE JOO CHANG, Department of Physics, KAIST — Despite considerable interests in transition metal dichalcogenides (TMDs), such as MX_2 with M = (Mo, W) and X = (S, Se, Te), the physical origin of their topological nature is still in its infancy. The conventional view of topological phase transition (TPT) in TMDs is that the band inversion occurs between the metal d and chalcogen p orbital bands. More precisely, the former is pulled down below the latter. Here we introduce an explicit scheme for analyzing TPT in topological materials and find that the TPT in TMDs is different from the conventional speculation. When the 1T phase undergoes a structural transformation to the 1T' phase in monolayer MX_2, the band topology changes from trivial to non-trivial, leading to the TPT. We discuss the exact role of the metal d and chalcogen p orbital bands during the TPT. Our finding would provide clear guidelines for understanding the topological nature not only in TMDs but also in other topological materials yet to be explored.

Duk-Hyun Choe
Department of Physics, KAIST

Date submitted: 22 Jan 2016 Electronic form version 1.4