Electronic and optical properties of monoclinic $MoTe_2$

Transition metal dichalcogenides (TMDs), together with metallic graphene and highly insulating hexagonal boron nitride, have recently attracted renewed interests as an important two-dimensional component of next-generation devices. In particular, polymorph engineering in group 6 TMDs, such as MX_2 with M=(Mo, W) and X=(S, Se, Te), has been an intriguing theme in science for more than 50 years; most researches have been conducted with semiconducting hexagonal (2H) phase, however other polymorphs have not been explored due to their inhomogeneous formation in limited areas.

In this talk, I will discuss on structural phase transition between hexagonal and stable monoclinic (distorted octahedral or 1T') phase in bulk single-crystalline $MoTe_2$, and an electronic phase transition between semi-metallic (bulk) and semiconducting (few-layered) 1T'-$MoTe_2$. The newly discovered 1T'-$MoTe_2$ exhibits a maximum carrier mobility of 4,000 $cm^2V^{-1}s^{-1}$ and a giant magnetoresistance of 16,000% in a magnetic field of 14 Tesla at 1.8 Kelvin in the bulk form, and the few-layered 1T'-$MoTe_2$ reveals a bandgap of up to 60 meV in monoclinic TMDs. Our density functional theory calculations identify strong interband spin-orbit coupling (SOC) as the origin of bandgap opening in the few-layered monoclinic $MoTe_2$. It will be shown that the Peierls distortion is a key mechanism to stabilize the monoclinic structure. This new class of semiconducting $MoTe_2$ unlocks the possibility of topological quantum devices based on nontrivial Z_2-band-topology quantum spin Hall insulators in monoclinic TMDs and low interface resistance 2D semiconductor devices.