Young-Woo Son
Affiliation: Korea Institute for Advanced Study, Seoul, Korea

Structural and electronic stability of transition metal dichalcogenides

In this talk, I will discuss a couple of novel interplays between structures and electronic properties of layered transition metal dichalcogenides (TMDs). Among several TMDs, three-dimensional MoTe2 and WTe2 share almost similar lattice constants as well as topological electronic properties except their structural phase transitions. While the former shows a well-known first order phase transition between monoclinic and orthorhombic structures, the latter does not. Using a state-of-the-art first-principles calculation method, we investigate their structural stability and uncover that the disparate phase transitions originate from delicate differences between their interlayer bonding states near the Fermi energy. By exploiting the relation between the structural phase transitions and the low energy topological electronic properties, we show that a charge doping can control the transition substantially, thereby suggesting a way to stabilize or to eliminate their topological electronic energy bands. I will also discuss the electronic phase diagram of the both materials as a function of external charge doping. I show that in low doping, enhanced electron-phonon interactions enhance the superconducting (SC) transition temperatures. As increasing doping density, the SC temperature gradually decreases to zero and then various new CDW states emerge. Physical origins of new collective phenomena will be briefly discussed.