

Abstract Submitted
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Electronic and structural phase transitions induced by uniaxial strains in monolayer SnSe YABEI WU, Shanghai University; University at Buffalo, SUNY, WEIWEI GAO, University at Buffalo, SUNY, PEIHONG ZHANG, Shanghai University; University at Buffalo, SUNY, WEI REN, Shanghai University — Two dimensional (2D) materials have attracted unprecedented research interest owing to their unique properties that are suitable for various applications. Recent research has started to explore 2D materials beyond graphene; examples include transition metal dichalcogenides and black phosphorus. Bulk SnSe is a layered semiconductor which exists in two phases. The low temperature Pnma phase has an indirect band gap of 0.89 eV and a direct band gap of 1.3 eV, while the high temperature Cmcm phase is stabilized at $T > 800$ K. In this talk, we will present first-principles investigations of the effects of strains on the electronic and structural properties of SnSe. We find that uniaxial strains are an effective means to tune the properties single layer SnSe, and may also induce phase transitions in this system.

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