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Tuning band gap of monolayer and bilayer SnS2 by strain effect and external electric field : A first principles calculations[1] ABEERA RAHMAN, YOUNG-HAN SHIN, University of Ulsan — Recently many efforts have been paid to two-dimensional layered metal dichalcogenides (LMDs). Among them MoS_2 has become a prototype LMD, and recent studies show surprising and rich new physics emerging in other van der Waals materials such as layered SnS_2 [1-4]. SnS_2 is a semiconducting earth-abundant material and Sn is a group IV element replacing the transition metal in MoS_2. SnS_2 shows new possibilities in various potential applications. However, the knowledge on basic properties of layered SnS_2 is still not well understood. In this study, we consider two types of structures; 1T with $P\bar{3}m1$ (164) space group and 1H with $P6_3/mmc$ (194) space group. Our first principles calculations show that the 1T structure for SnS_2 is more stable than the 1H structure whereas latter is more stable for MoS_2. Moreover,in contrast to MoS_2,SnS_2 shows an indirect band gap both for 1T and 1H structures while 1T MoS_2 is metallic and 1H has a direct band gap. We also study strain effect in the range of 0-10% on the band structure for monolayer and bilayer SnS_2 (both for 1T and 1H structures).We find significant change in their band gaps. We also investigate the bilayer SnS_2 with and without out-of-plane stress.

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