

Abstract Submitted
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Bonding Directionality Matters: Direct-Indirect Transition in Few-Layer SnSe. HANSIKA SIRIKUMARA, THUSHARI JAYASEKERA, Southern IL Univ-Carbondale — SnSe is one of the best thermoelectric materials reported to date. The possibility of growing few-layer SnSe helped boost the interest in SnSe, and paves the path for various other applications such as photovoltaics and optoelectronics. However, indirect band gap of SnSe hinders its success in such fields. Based on the results from first principles Density Functional Theory, we carefully analyzed electronic band structures of bulk, mono and few-layer SnSe with various interlayer stackings. Our results reveal that it is the directionality of interlayer interactions, which leads to the indirect electronic band gap. In fact, by modifying the interface between layers, there is a possibility of achieving few-layer SnSe with direct electronic band gap. Moreover, the fundamental understanding of interlayer interactions at the atomic level also paves the path for designing Van der Waals heterostructures based on SnSe with prescribed electronic properties.

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