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Strain Dependent Direct Indirect Band Gap Transition in Tin Monochalcogenide Heterostructures JAVAD AZADANI, University of Minnesota, ONGUN OZCELIK, Princeton University, MOHAMMAD FATHI , University of Southern California, TONY LOW, tlow@umn.edu — We present a comprehensive study of the electronic and mechanical properties of SnS-SnSe heterostructures. Based on first-principles density functional calculations, we show that SnS and SnSe layers can form hetetrostructures with diverse properties depending on the stacking and the geometrical phases of its constituent monolayers. In particular, the heterostructure created from the puckered phases of SnS and SnSe monolayers have strain dependent electronic and mechanical properties. The band gap of this material can be tuned and changed from direct to indirect by applying strain in zigzag and armchair directions. Moreover, the applied strain can also change the sliding barrier of the monolayers on top of each other giving rise to super lubricity at certain strain values.

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