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Puckering Inversion in Monolayer Group IV Monochalcogenides SnS and GeSe Through Strain Engineering PAUL HANAKATA, Boston University, ALEXANDRA CARVALHO, National University of Singapore, DAVID CAMPBELL, HAROLD PARK, Boston University — .We use first principles calculations to study the electronic and mechanical properties of the monolayer group IV monochalcogenides SnS and GeSe under uniaxial stress in the armchair or zigzag direction. We find that monolayer SnS and GeSe can sustain tensile stresses up to 3.5 GPa and 7 GPa, respectively. Applying uniaxial stress in the zigzag direction results in a structural phase transition to a rocksalt-like structure for both GeSe and SnS and followed by an inversion in the puckering structure. This puckering inversion results in a change of the band structure, in particular the valley configuration. Our findings show the potential applications of SnS and GeSe monolayer for phase-change memory and valley-based electronic devices.

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