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Layer-dependent electronic and vibrational properties of SnSe₂ and SnS₂ 2D materials JOSEPH GONZALEZ, RUDY SCHALF, IVAN OLEYNIK, University of South Florida — Layered metal chalcogenides possess a wide range of unique electronic properties, which are currently explored for applications as novel two-dimensional electronic materials. SnS₂ and SnSe₂ layered materials consist of covalently bonded S-Se-S (Sn-Se-Sn) sheets bonded together by weak van der Waals interactions. The atomic, electronic and vibrational properties of SnS₂ and SnSe₂ thin films are investigated using first-principles density functional theory. The evolution of the thickness-dependent band structure and Raman spectra are discussed, as well as the effects of strain and the influence of the substrate. The first-principles results are compared with available experimental data.

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