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Structural, electronic and vibrational properties of few-layer 2H- and 1T-$TaSe_2$[1] JIA-AN YAN, MACK DELA CRUZ, Department of Physics, Astronomy and Geosciences, Towson University, BRANDON COOK, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN, 37831 USA, KALMAN VARGA, Department of Physics and Astronomy, Vanderbilt University, Nashville, Tennessee 37235, USA — Two-dimensional metallic transition metal dichalcogenides (TMDs) are of interest for studying phenomena such as charge-density wave (CDW) and superconductivity. Few-layer tantalum diselenides ($TaSe_2$) are typical metallic TMDs exhibiting rich CDW phase transitions. However, a description of the structural, electronic and vibrational properties for different crystal phases and stacking configurations, essential for interpretation of experiments, is lacking. We present first-principles calculations of structural phase energetics, band dispersion near the Fermi level, phonon properties and vibrational modes at the Brillouin zone center for different layer numbers, crystal phases and stacking geometries. Evolution of the Fermi surfaces as well as the phonon dispersions as a function of layer number reveals dramatic dimensionality effects in this CDW material. Our results indicate strong electronic interlayer coupling, detail energetically possible stacking geometries, and provide a basis for interpretation of Raman spectra.

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