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First-principles study of monolayer and bilayer $TaSe_2$[1] MACK ADRIAN DELA CRUZ, JIA-AN YAN, Department of Physics, Astronomy and Geosciences, Towson University — Two-dimensional atomic crystals of transition metal dichalcogenides (such as MoS_2, $TaSe_2$, etc.) are currently attracting growing attention due to the broad variety of electronic properties presented in these systems. Here we present a first-principles study of the structural, electronic and vibrational properties of monolayer and bilayer $TaSe_2$, which is a charge-density wave material in the bulk form. The structure of monolayer $TaSe_2$ is determined by performing a series of total energy calculations. For bilayer $TaSe_2$, various stackings of monolayer $TaSe_2$ with the hexagonal (2H) and the trigonal (1T) phases, will be considered. Calculated electronic and phonon properties of the energetically favorable states will be compared with the available experimental data.

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