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Electronic and vibrational properties of monolayer and bilayer $TaSe_2$[1] MACK ADRIAN DELA CRUZ[2], JIA-AN YAN, Department of Physics, Astronomy, Geosciences, Towson University — Distinct from MoS_2, two-dimensional atomic crystal of tantalum diselenide ($TaSe_2$) is metallic and exhibits charge-density wave (CDW) transitions. Using density-functional theory, we present a first-principles study of the electronic and vibrational properties of monolayer and bilayer $TaSe_2$ without including the CDW-induced structural distortions. For monolayer 1T-$TaSe_2$, the frequencies of the Raman active modes are 159 cm^{-1} (E_g) and 226 cm^{-1} (A_{1g}), while the Raman-active modes for monolayer 2H-$TaSe_2$ are at 138 cm^{-1} (E''), 214 cm^{-1} (E'), and 241 cm^{-1} (A_1'). For bilayer $TaSe_2$, different stackings of monolayer 2H-$TaSe_2$ and 1T-$TaSe_2$ phases have been calculated. Electronic band structures and vibrational properties of four energetically favorable configurations will be presented. Finally, the spin-orbit coupling on the structural and electronic properties will also be discussed.

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