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Interplane and Intraplane Coupling in Charge-Density-Wave Phases of 1T-TaS_2 and 1T-$TaSe_2$ YIZHI GE, AMY LIU, Georgetown University — At low temperatures, the layered transition metal dichalcogenides 1T-TaS_2 and 1T-$TaSe_2$ adopt similar charge-density wave structures corresponding to a $\sqrt{13}\times\sqrt{13}$ reconstruction in which the Ta atoms cluster within the triangular layers. Yet TaS_2 also undergoes a metal-insulator transition, while $TaSe_2$does not. Here we present a density-functional-theory study of the electronic structure of 1T-TaS_2 and 1T-$TaSe_2$. The half filled Ta d band at the Fermi level is found to differ significantly in the two materials: in $TaSe_2$ the band is three dimensional, while in TaS_2 it is highly one dimensional. These results are analyzed using maximally localized Wannier functions. The effects of stacking sequence and the spin-orbit interaction will also be discussed.

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