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Effect of dimensionality on charge density wave instabilities in TaS₂ and TaSe₂ YIZHI GE, AMY Y. LIU, Physics Department, Georgetown University — Recent successes in making exfoliated single-layer transition-metal dichalcogenides has brought new interest to these materials, particularly with respect to the effects of dimensionality. As layered bulk materials, the 1T and 2H polymorphs of TaS₂ and TaSe₂ undergo a number of charge-density-wave (CDW) transitions. However, recent experiments have found that the CDW instability does not survive in nanopatches of 2H-TaS₂. Here we present a density-functional theory investigation of the CDW instability in single- and few-layer TaS₂ and TaSe₂, focusing on the role of the interlayer interactions. The effects of dimensionality on structure, electronic structure, and electronic-phonon coupling will be discussed.

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