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Charge-density-wave and superconducting instabilities in TaS₂ and TaSe₂ YIZHI GE, AMY LIU, Physics Department, Georgetown University — At ambient pressure, 1T-TaS₂ and 1T-TaSe₂ undergo similar charge-density-wave transitions at low temperature. Recent experiments have further found that 1T-TaS₂ becomes superconducting under pressure. Here we present density-functional theory investigations of the CDW and superconducting instabilities in these two materials. The calculations, which accurately capture the instability of the undistorted 1T structure at zero pressure, confirm that pressure suppresses the CDW instability in both materials. The calculated electron-phonon coupling constants in the compressed phases show strong wave-vector dependence and are large enough to suggest that both materials should have superconducting phases under pressure. The relationship between the CDW instability, Fermi surface topology, and electron-phonon coupling will also be discussed.

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