

Abstract Submitted
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Zone-center phonons of bulk, few-layer, and monolayer 1T-TaS₂: Application to Raman scattering¹ OLIVER R ALBERTINI, Georgetown University, RUI ZHAO, Pennsylvania State University, REBECCA L MCCANN, Georgetown University, SIMIN FENG, MAURICIO TERRONES, Pennsylvania State University, JAMES K FREERICKS, Georgetown University, JOSHUA A ROBINSON, Pennsylvania State University, AMY Y LIU, Georgetown University — The transition metal dichalcogenide 1T-TaS₂ has attracted attention for decades due to its multiple charge density wave phases. More recently it is being considered as a 2D device material, due to the wide range of electrical conductivities in these phases. The metal-insulator transition that occurs when the commensurate charge density wave forms is particularly attractive. We present first-principles calculations of the vibrational properties of 1T-TaS₂ for various thicknesses in the high-temperature (undistorted) phase and the low-temperature commensurate charge density wave phase. We also present measurements of the Raman frequencies for bulk and few-layer samples in the low-T phase. We find strong evidence for the low-T commensurate charge density wave state remaining stable as the crystal is thinned, even down to one layer. We explore the effects of substrate-induced strain on the vibrational spectrum and propose polarized Raman spectroscopy as a method for quickly identifying the c-axis orbital texture in the low-T phase. This orbital texture has recently been identified as playing a role in the metal-insulator transition.

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