Abstract Submitted
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Spin polarization driven by a charge-density wave in monolayer 1T-TaS_2[1] QINGYUN ZHANG, LI-YONG GAN, YINGCHUN CHENG, UDO SCHWINGENSCHLOGL, Physical Sciences and Engineering, King Abdullah University of Science and Technology, COMPUTATIONAL PHYSICS AND MATERIALS SCIENCE TEAM — Using first-principles calculations, we investigate the electronic and vibrational properties of monolayer T-phase TaS_2. Our results demonstrate that the formation of a CDW is energetically favorable at low temperature, similar to bulk 1T-TaS_2. Electron-phonon coupling is found to be essential for the lattice reconstruction. In the CDW phase the electronic states near the Fermi level are strongly localized, which explains the formation of significant magnetic moments. The spin polarization transforms the material into a magnetic semiconductor. The combination of inherent spin polarization with a semiconducting nature distinguishes the monolayer fundamentally from the bulk compound as well as from other two-dimensional transition metal dichalcogenides. Monolayer T-phase TaS_2 therefore has the potential to enable two-dimensional spintronics.

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