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Magnetism and Raman Spectroscopy of Pristine and Hydrogenated TaSe2 Monolayer tuned by Tensile and Pure Shear Strain SUGATA CHOWDHURY, The Catholic University of America, Washington DC National Institute of Standards and Technology, MD, JEFFREY SIMPSON, Towson University, MD National Institute of Standards and Technology, MD, T. L. EINSTEIN, Univ of Maryland-College Park, ANGELA R. HIGHT WALKER, National Institute of Standards and Technology, MD — 2D-materials with controllable optical, electronic and magnetic properties are desirable for novel nanodevices. Here we studied these properties for both pristine and hydrogenated TaSe2 (TaSe2-H) monolayer (ML) in the framework of DFT using the PAW method. We considered uniaxial and biaxial tensile strain, as well as shear strain along the basal planes in the range between 1% and 16%. Previous theoretical works (e.g. APL 107, 032402 (2015)) considered only symmetrical biaxial tensile. Pristine ML is ferromagnetic for uniaxial tensile strain along $\hat{x}$ or $\hat{y}$. For tensile strain in $\hat{y}$, the calculated magnetic moments of the Ta atoms are twice those for the same strain in $\hat{x}$. Under pure shear strain (expansion along $\hat{y}$ and compression along $\hat{x}$), a pristine ML is ferromagnetic, but becomes non-magnetic when the strain directions are interchanged. Due to carrier-mediated double-exchange, the pristine ML is ferromagnetic when the Se-Ta-Se bond angle is $< 82°$ and the ML thickness is < 3.25Å. We find that all Raman-active phonon modes show obvious red-shifting due to bond elongation and the E2 modes degeneracy is lifted as strain increases. For a TaSe2-H ML, the same trends were observed. Results show the ability to tune the properties of 2D-materials.

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