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Probing the uniaxial strains in MoS_2 using polarized Raman spectroscopy: A first-principles study[1] DANNA DORATOTAJ, JEFFREY R. SIMPSON, JIA-AN YAN, Towson University — Characterization of strain in two-dimensional crystals is important for understanding their properties and performance. Using first-principles calculations, we study the effects of uniaxial strain on the Raman-active modes in monolayer MoS_2. We show that the in-plane E' mode at 384 cm^{-1} and the out-of-plane A_1' mode at 403 cm^{-1} can serve as fingerprints for the uniaxial strain in this material. Specifically, under a uniaxial strain, the doubly degenerate E' mode splits into two non-degenerate modes: the $E'_{||}$ and $E'_{\perp}$ modes. The frequency of the $E'_{||}$ mode blue-shifts for a compressive strain, but red-shifts for a tensile strain. In addition, due to the strain-induced anisotropy in the MoS_2 lattice, the polarized Raman spectra of the $E'_{||}$ and $E'_{\perp}$ modes exhibit distinct angular dependence for specific laser polarization setups, allowing for a precise determination of the direction of the strain with respect to the crystallographic orientation. Furthermore, we find that the polarized Raman intensity of the A_1' mode also shows evident dependence on the applied strain, providing additional effective clues for determining the direction of the strain even without knowledge of the crystallographic orientation. Thus, polarized Raman spectroscopy offers an efficient non-destructive way to characterize the uniaxial strains in monolayer MoS_2.

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