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Probing the uniaxial strains in MoS_2 using polarized Raman spectroscopy: A first-principles study DANNA DORATOTAJ, JIA-AN YAN, Department of Physics, Astronomy, and Geosciences, Towson University, 8000 York Road, Towson, MD 21252, USA — Characterization of strain in two-dimensional (2D) crystals is important for understanding their properties and performance. Using first-principles calculations, we study 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} can serve as a fingerprint for the uniaxial strain in this 2D material. Specifically, under a uniaxial strain, the doubly degenerate E' mode splits into two non-degenerate modes: one is $E'_{\parallel}$ mode in which atoms vibrate in parallel to the strain direction, and the other is $E'_{\perp}$ mode in which atoms vibrate perpendicular to the strain direction. The frequency of the $E'_{\parallel}$ 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 $E'_{\parallel}$ and $E'_{\perp}$ modes exhibit distinct angular dependence, allowing for a precise determination of the direction of the uniaxial strain. Thus, the polarized Raman spectroscopy offers an efficient non-destructive way to characterize the uniaxial strains in monolayer MoS_2.

Danna Dora
Department of Physics, Astronomy, and Geosciences, Towson University, 8000 York Road, Towson, MD 21252,

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