

# Investigation of Optical and Vibrational Properties of monolayer $\text{Mo}_{1-x}\text{Nb}_x\text{S}_2$ ternary alloys grown by MOCVD

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## Abstract

Band gap engineering of monolayer transition metal dichalcogenides is indispensable to tailoring the functionalities, manipulate the emission properties and create countless combinations of heterostructures with different band offsets for potential use in solar cells, photodetectors, phototransistors and valley spintronics. Here, we present a detailed study on the controlled synthesis of  $\text{Mo}_{1-x}\text{Nb}_x\text{S}_2$  monolayer alloys, with compositions ranging from  $x = 0$  to 0.67 using metal organic (MOCVD) chemical vapor deposition. The formation of ternary  $\text{Mo}_{1-x}\text{Nb}_x\text{S}_2$  alloys and the associated strain resulting from alloying were demonstrated through a combination of optical spectroscopy and XPS characterization techniques. Our finding suggest that defects like dimers, vacancies, and metal dopant substantially induced FWHM and induce a larger red shift in the alloy films, as confirmed by Raman spectroscopy. A lattice tensile strain ( $\sim 0.58\%$ ) and compressive strain ( $\sim 1.25\%$ ) was estimated when the Nb atom substituted in the  $\text{MoS}_2$  lattice calculated utilizing Raman spectroscopy. Furthermore, we investigate the impact of alloying mediated strain on optical absorption and emission behavior, particularly trions and impurity-bound excitons in monolayer  $\text{Mo}_{1-x}\text{Nb}_x\text{S}_2$  ternary alloys.

## References:

1. Schulpen JJ et al. ACS Applied Nano Materials. 2024 Apr 1;7(7):7395-407
2. Song B et al. ACS Applied Electronic Materials. 2021 May 26;3(6):2564-72

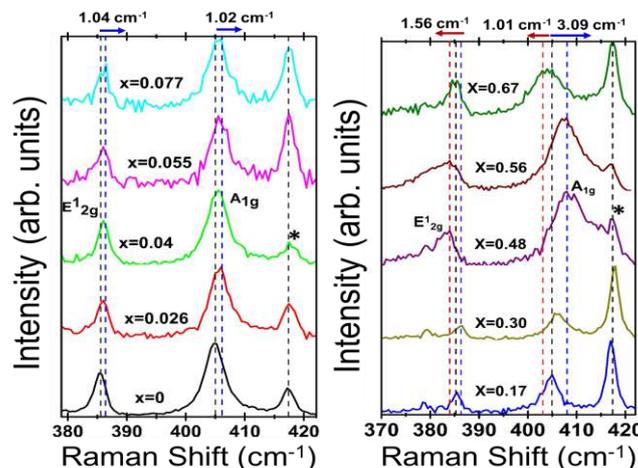


Figure 1. Raman spectra of  $\text{Mo}_{1-x}\text{Nb}_x\text{S}_2$  monolayer alloy with different Nb concentrations.