Stacking-Dependent Optical Properties in Bilayer WSe_2

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It has recently been demonstrated that the angle between layers of two-dimensional materials can strongly impact the resulting properties, inspiring the rapidly developing research area of twistronics. Here, we investigate stacking-dependent optical properties in bilayer WSe_2.[1] Both 2H and 3R stacking orientations are synthesized by chemical vapor deposition. Samples are investigated using photoluminescence, Raman spectroscopy, and reflectivity measurements under ambient and cryogenic conditions. In both 2H and 3R systems, the A_{1g} Raman mode is sensitive to excitation conditions, with orders of magnitude enhancement observed for certain excitation wavelengths. However, the laser wavelength leading to maximum enhancement is distinctly different for the two stacking orientations, with 2H-WSe_2 exhibiting maximum enhancement under 514 nm excitation and 3R-WSe_2 at 520 nm excitation at cryogenic temperatures. DFT calculations and reflectivity measurements indicate differences in band structure between the two systems, evident by shifts in emission energy of excitonic features, and elucidate the source of variation in Raman spectra. Maximum Raman enhancement is achieved when the excitation wavelength is resonant with the stacking-dependent C-excitonic feature. This work provides a comprehensive investigation of optical properties in 2H- and 3R-WSe_2 bilayers.

[1] K. M. McCreary *et al.*, "Stacking-dependent optical properties in bilayer WSe_2," *Nanoscale*, vol. 14, no. 1, pp. 147–156, 2022, doi: 10.1039/D1NR06119D.