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Ultralow-frequency interlayer Raman modes to probe interfacial coupling in twisted bilayer MoS_2[1] SHENGXI HUANG, MIT, LIANGBO LIANG, RPI, ORNL, XI LING, MIT, ALEXANDER PURETZKY, DAVID GEOHEGAN, BOBBY SUMPTER, ORNL, JING KONG, MIT, VINCENT MEUNIER, RPI, MILDRED DRESSELHAUS, MIT — Interlayer coupling strength plays an important role in tuning the optoelectronic properties of transition metal dichalcogenides (TMDs), which can be studied in twisted bilayer TMDs due to their various stacking configurations. In this work, ultralow-frequency interlayer shear and breathing Raman modes were investigated in twisted bilayer MoS_2. We found both twisted angle and translational shift can significantly influence the interlayer coupling, leading to notable frequency and intensity changes of low-frequency Raman modes, as confirmed by first-principles density functional theory calculations. Large frequency and intensity variations occur near twisted angles $0^o$and 60^o, but not between $20^o$and 40^o, indicating translational shift does not induce much change of the coupling strength within the latter angle range. In contrast to low-frequency interlayer modes, high-frequency intralayer Raman modes are much less sensitive to interlayer coupling. Therefore, interlayer Raman modes can be used as an effective probe to study the interlayer coupling of 2D materials with different stacking configurations.

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