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Low-frequency Raman modes as fingerprints of layer stacking configurations of transition metal dichalcogenides[1] LIANGBO LIANG, ALEXANDER PURETZKY, BOBBY SUMPTER, Oak Ridge National Lab, VINCENT MEUNIER, Rensselaer Polytechnic Institute, DAVID GEOHEGAN, Oak Ridge National Lab, DAVID B. GEOHEGAN TEAM, VINCENT MEUNIER TEAM — The tunable optoelectronic properties of stacked two-dimensional (2D) crystal monolayers are determined by their stacking orientation, order, and atomic registry. Atomic-resolution Z-contrast scanning transmission electron microscopy (AR-Z-STEM) can be used to determine the exact atomic registration between different layers in few-layer 2D stacks; however, fast and relatively inexpensive optical characterization techniques are essential for rapid development of the field. Using two- and three-layer MoSe2 and WSe2 crystals synthesized by chemical vapor deposition, we show that the generally unexplored low-frequency (LF) Raman modes (¡50 cm-1) that originate from interlayer vibrations can serve as fingerprints to characterize not only the number of layers, but also their stacking configurations [Puretzky and Liang et al, ACS Nano 2015, 9, 6333]. First-principles Raman calculations and group theory analysis corroborate the experimental assignments determined by AR-Z-STEM and show that the calculated LF mode fingerprints are related to the 2D crystal symmetries. Our combined experimental/theoretical work demonstrates the LF Raman modes potentially more effective than HF Raman modes to probe the layer stacking and interlayer interaction for 2D materials.

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