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First-principles study of low-frequency phonon modes in heterostructures of transition metal dichalcogenides[1] NATHAN PRINS, DANNA DORATOTAJ, JIA-AN YAN, Towson University — Transition metal dichalcogenides (TMDs) are layered compounds with weak interlayer interactions and have attracted tremendous attention because of their remarkable electronic, optical and transport properties. Heterostructures made of TMDs offer an additional degree of freedom to tune their electronic properties. In this work, we present a first-principles study of the low-frequency modes in WS_2/MoS_2 and $WSe_2/MoSe_2$ heterostructures for various stacking geometry and stacking sequence. Our calculations show that the low-frequency layer shearing modes and layer breathing modes provide a useful way to characterize the stacking geometry of these heterostructures. Finally, the simulated Raman spectra for these heterostructures are discussed.

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