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Phonon Properties in 2D Transition Metal Dichalcogenide Crystals: Symmetry and Dimensionality Matter YANYUAN ZHAO, Nanyang Technological University, Singapore, XIN LUO, Institute of High Performance Computing, Singapore, HAI LI, Nanyang Technological University, Singapore, PAULO ARAUJO, Massachusetts Institute of Technology, HUA ZHANG, Nanyang Technological University, Singapore, SU YING QUEK, Institute of High Performance Computing, Singapore, MILDRED DRESSELHAUS, Massachusetts Institute of Technology, JUN ZHANG, QIHUA XIONG, Nanyang Technological University, Singapore — 2D transition-metal dichalcogenide (TMD) crystals possess lower symmetry compared to their bulk counterparts and thus have different phonon modes and behaviors. While in general the Raman active modes in 3D are also Raman active in 2D, the reverse is not always true due to the reduced symmetry in 2D. Here, using both Raman spectroscopy and first principles calculations, we uncover the ultra-low frequency ($5 \sim 55 \text{ cm}^{-1}$) interlayer breathing and shear modes in few-layer MoS_2 , MoSe_2 , WS_2 and WSe_2 , prototypical layered TMDs. The interlayer breathing modes correspond to an optically inactive mode in the bulk, and thus only exist in the 2D case. Remarkably, the frequencies of these modes can be perfectly described using a simple linear chain model. Besides, two new Raman peaks located at 176 cm^{-1} and 310 cm^{-1} were observed ONLY in few-layer WSe_2 , as a result of the lower symmetry in 2D. Our results shed light on a general understanding of the Raman/IR activities of the phonon modes in layered TMD materials and their evolution behaviors from 3D to the 2D.

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