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Predictive models for low-frequency Raman scattering in 2D materials

Two-dimensional (2D) layered materials have been extensively studied owing to their fascinating and technologically relevant properties. Their functionalities can be often tailored by the thickness and stacking. A quick, non-destructive and inexpensive tool is highly desirable for thickness and stacking characterization of 2D materials. Recently, low-frequency (LF) Raman spectroscopy quickly rises up as such tool, since LF interlayer modes, including the shear and breathing modes, are much more sensitive to the interlayer coupling compared to the typically studied high-frequency (HF) intralayer Raman modes [1,2,3]. The frequencies of LF modes are sensitive to the number of layers, which is explained by a linear chain model [1,2]. Meanwhile, the intensities of LF modes are sensitive to the stacking pattern [4,5]. We proposed a simple and generalized interlayer bond polarizability model [2] to explain and predict how the LF Raman intensities depend on complex stacking sequences for any thickness in a broad array of 2D materials, including graphene, MoS_2, $MoSe_2$, WSe_2, $NbSe_2$, $PdSe_2$, Bi_2Se_3, GaSe, h-BN, etc. Additionally, a general strategy is proposed to unify the stacking nomenclature for these 2D materials. Our model reveals the fundamental mechanism of LF Raman response to the thickness and stacking, and provides general rules for thickness and stacking identification of 2D materials.

References

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Figures

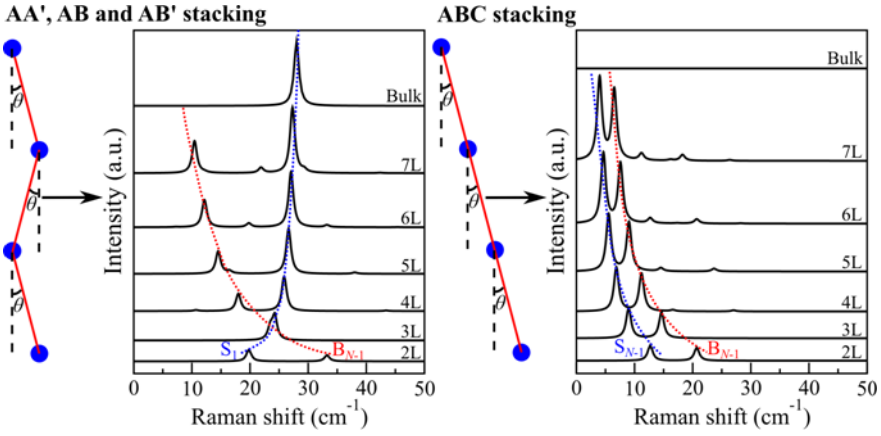

Figure 1: Calculated low-frequency Raman scattering of 2D materials for different stacking configurations at different number of layers, based on the interlayer bond polarizability model [2].