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Low-frequency interlayer breathing mode in few-layer black phosphorus XI LING, SHENGXI HUANG, MIT, LIANGBO LIANG, VINCENT ME-UNIER, RPI, MILDRED DRESSELHAUS, MIT — Black phosphorus (BP), as a layered material, has attracted intense interest recently. Many interesting electronic and optoelectronic properties are being explored based on its unique anisotropic structure. In this work, we studied the Raman spectra in few-layer BP, including the intralayer and interlayer vibrational modes. Besides the three typical Raman modes A_g^1 (~ 359 cm⁻¹), B_{2g} (~ 437 cm⁻¹), and A_g^2 (~ 466 cm⁻¹), low-frequency modes were observed in few-layer BP, as predicted by the first-principles density functional theory (DFT) calculation. The interlayer breathing mode at around 87 cm⁻¹ was assigned as A_g^0 , since the DFT calculation result showed it has the symmetry of A_g^0 . In addition, the polarization dependence of the Raman modes in BP is studied systematically. Both the DFT calculation and the experimental results show that the polarization dependence profiles are sensitive to the crystal orientation of BP. In addition, the temperature dependence of the modes is studied in the range of -150 °C to room temperature. It is found that the A_q^0 mode has almost no dependence on the temperature change, and the out-of-plane mode (A_q^1) has weaker dependence than the in-plane modes $(B_{2g} \text{ and } A_q^2)$.

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