Phonon confinement effect in two-dimensional nanocrystals

of black phosphorus with anisotropic phonon dispersions†

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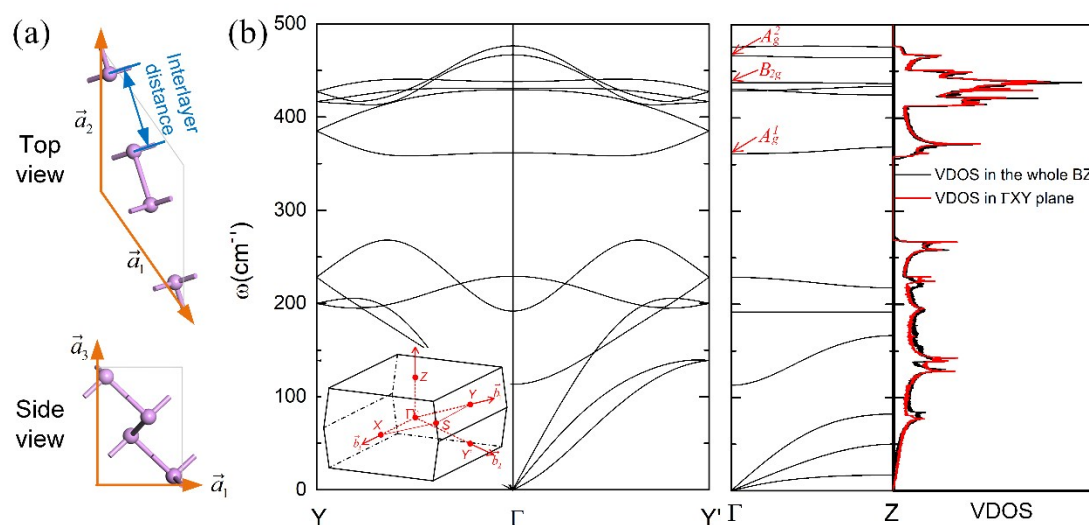* E-mail: liuxuelu@semi.ac.cn, phtan@semi.ac.cn

Fig. S1. (a) The unit cell of bulk BP with top and side view, where $\vec{a}_1, \vec{a}_2$ and $\vec{a}_3$ indicate lattice vectors. (b) Phonon dispersion of bulk BP and vibrational density of states (VDOS) in ΓXY plane (red) and the whole BZ (black). The insert shows BZ of the unit cell, where $\vec{b}_1, \vec{b}_2$ and $\vec{b}_3$ indicate reciprocal lattice vectors. VDOS in ΓXY plane and in the whole BZ show a little discrepancy in low frequency range ($\omega < 300 cm^{-1}$), while they are almost the same in the high frequency range ($\omega > 300 cm^{-1}$).
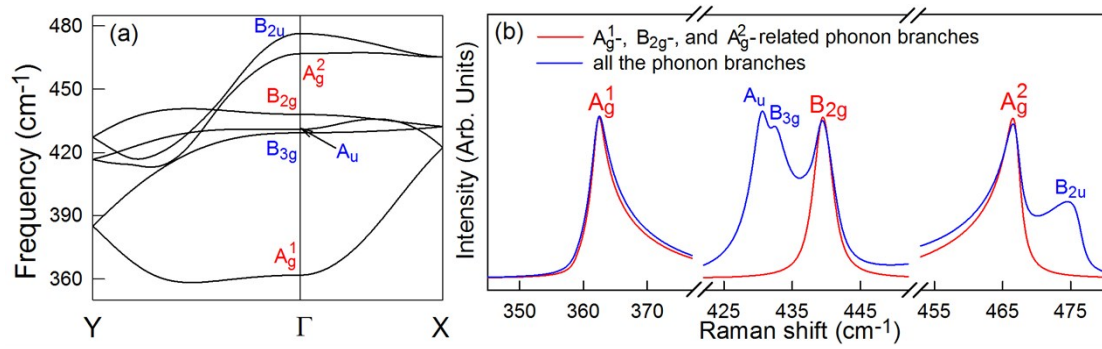
Fig. S2 (a) Phonon dispersion along ΓX and ΓY directions, and the vibration modes at Γ point are divided into Raman active (red) and inactive (blue) modes. (b) Line shape of Raman modes considering the contributions from the A_{g-}^2, B_{2g-} and A_{g-}^1related phonon branches (red) and that from all the phonon branches (blue). Both of two profiles are stimulated with L_D=2nm, α=18. In the latter line shape, additional peaks appear, which are contributed from phonon branches related with Raman-inactive modes at Γ point, i.e., A_u, B_{3g} and B_{2u}. Actually, the additional peaks related with Raman-inactive modes cannot be observed in the Raman spectra.