Supporting Information For

Two-dimensional Be_2Al and Be_2Ga monolayer: an anti-van′t Hoff/Le Bel planar hexacoordinate bonding and superconductivity

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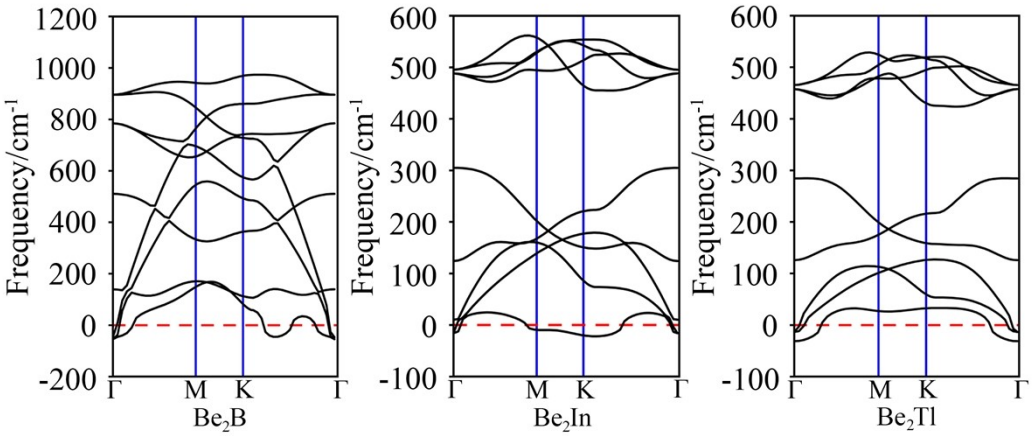

Figure S1. Phonon dispersion of the Be_2B, Be_2In, and Be_2Tl monolayers.

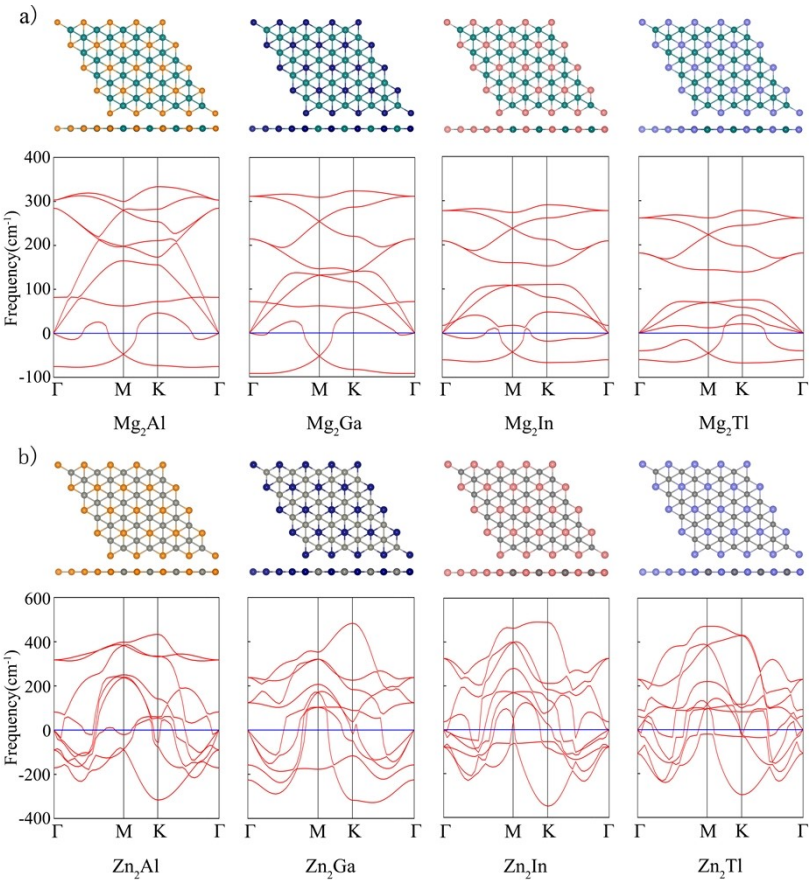

Figure S2. The crystal structure of Ae_2M (Ae = Mg, Zn; M = Al, Ga) monolayer and the corresponding phonon dispersion curves.

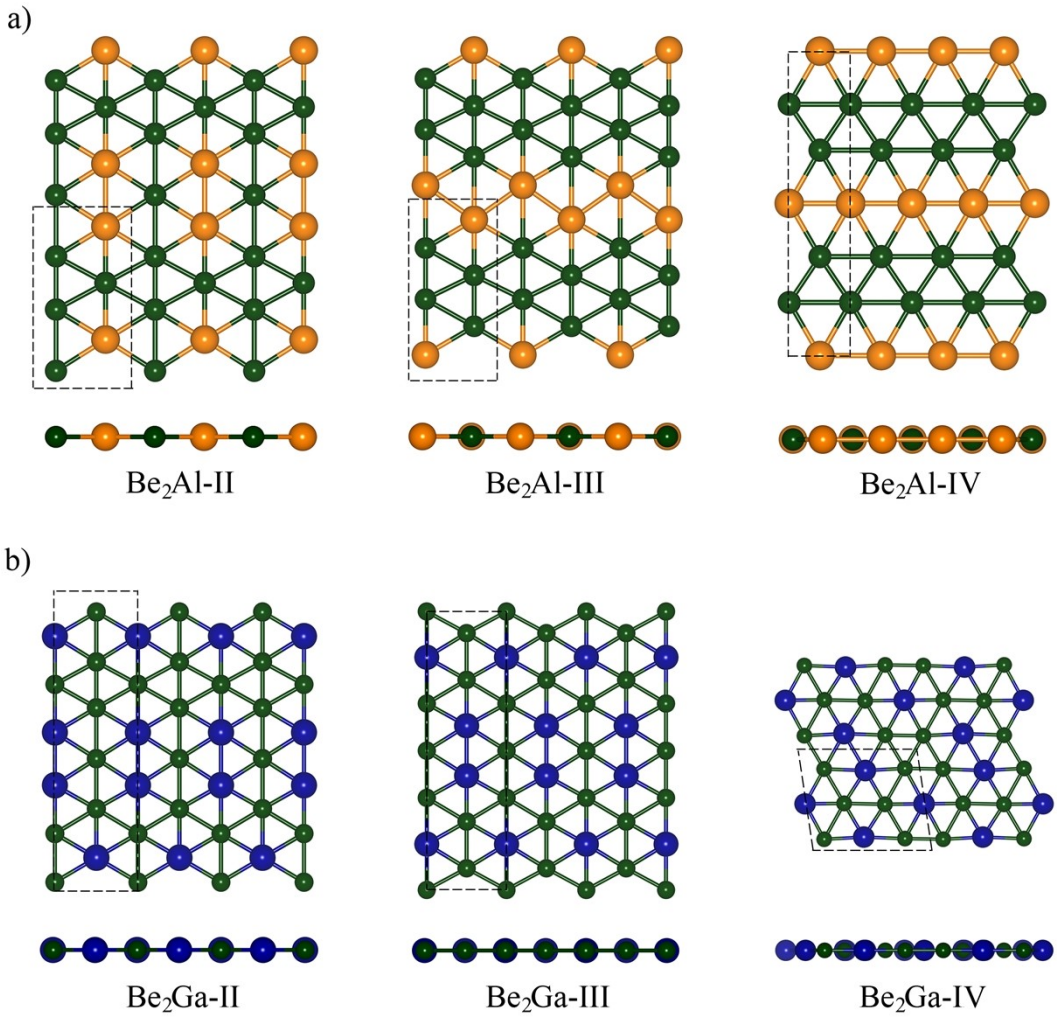

Figure S3. Top and side views of low-lying structures of a) Be_2Al and b) Be_2Ga 2D monolayers confirmed by particle swarm searches. The green, yellow, and blue balls represent Be, Al, and Ga atoms, respectively.

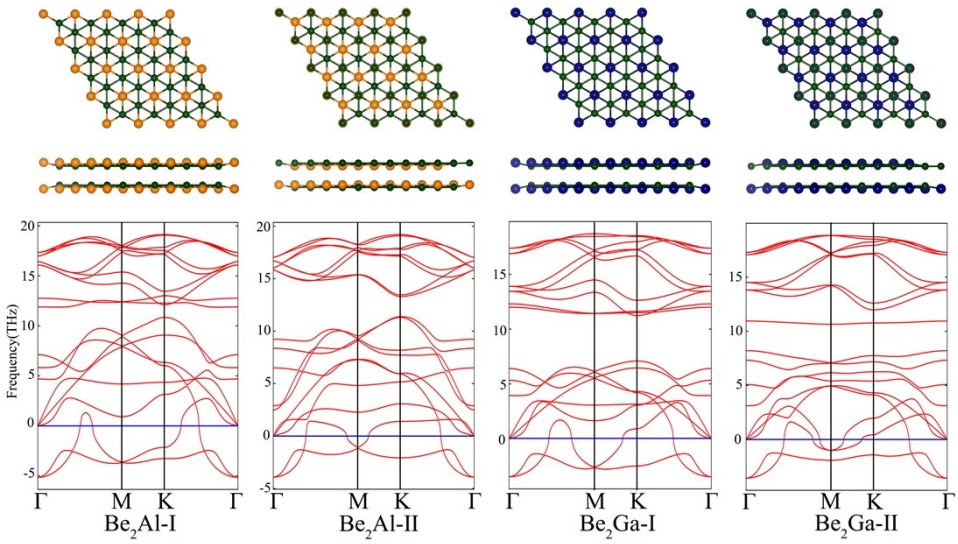

Figure S4. The crystal structure and phonon dispersion curves of Be_2M (M = Al, Ga) bilayer.

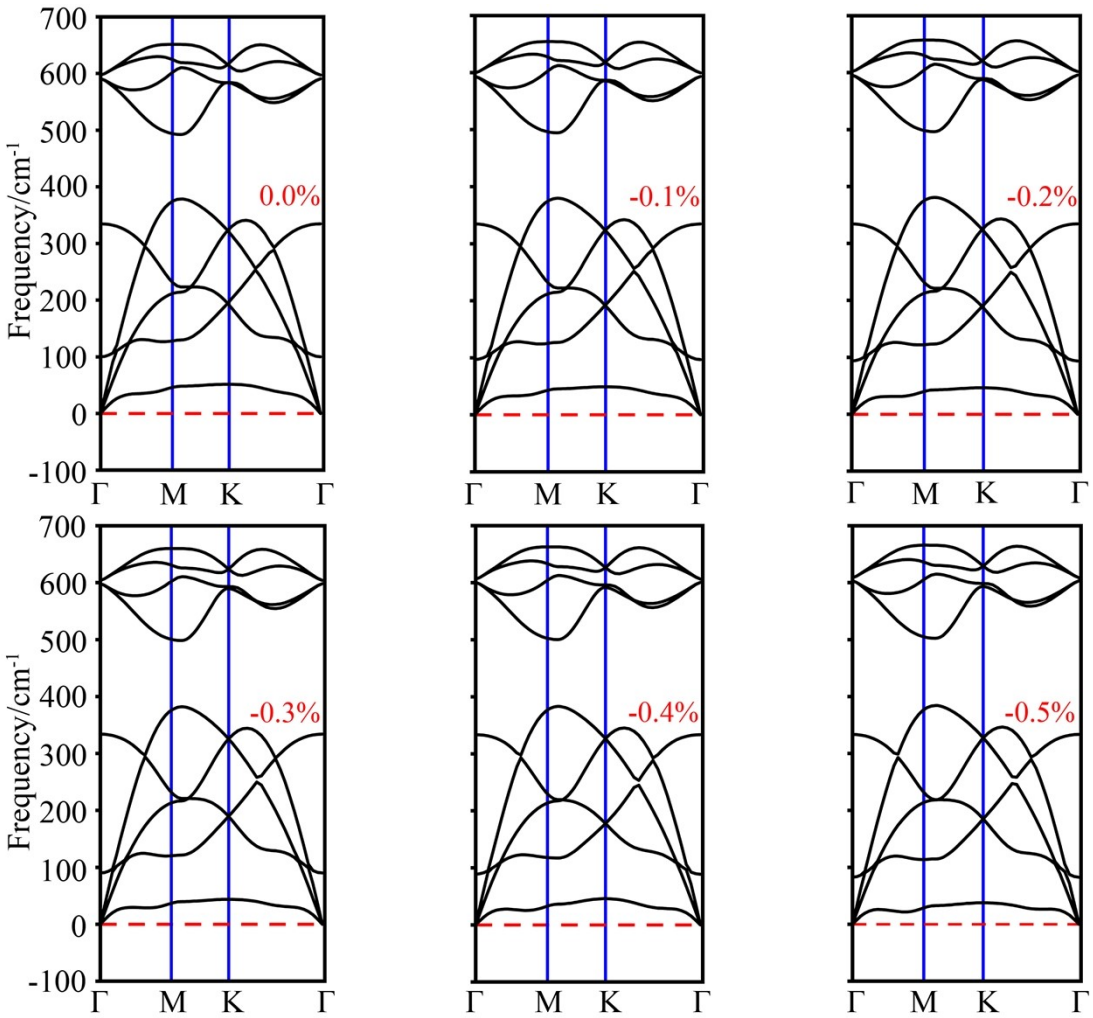

Figure S5. Phonon dispersion spectra of Be_2Al under strain from -0.5% to 0%.

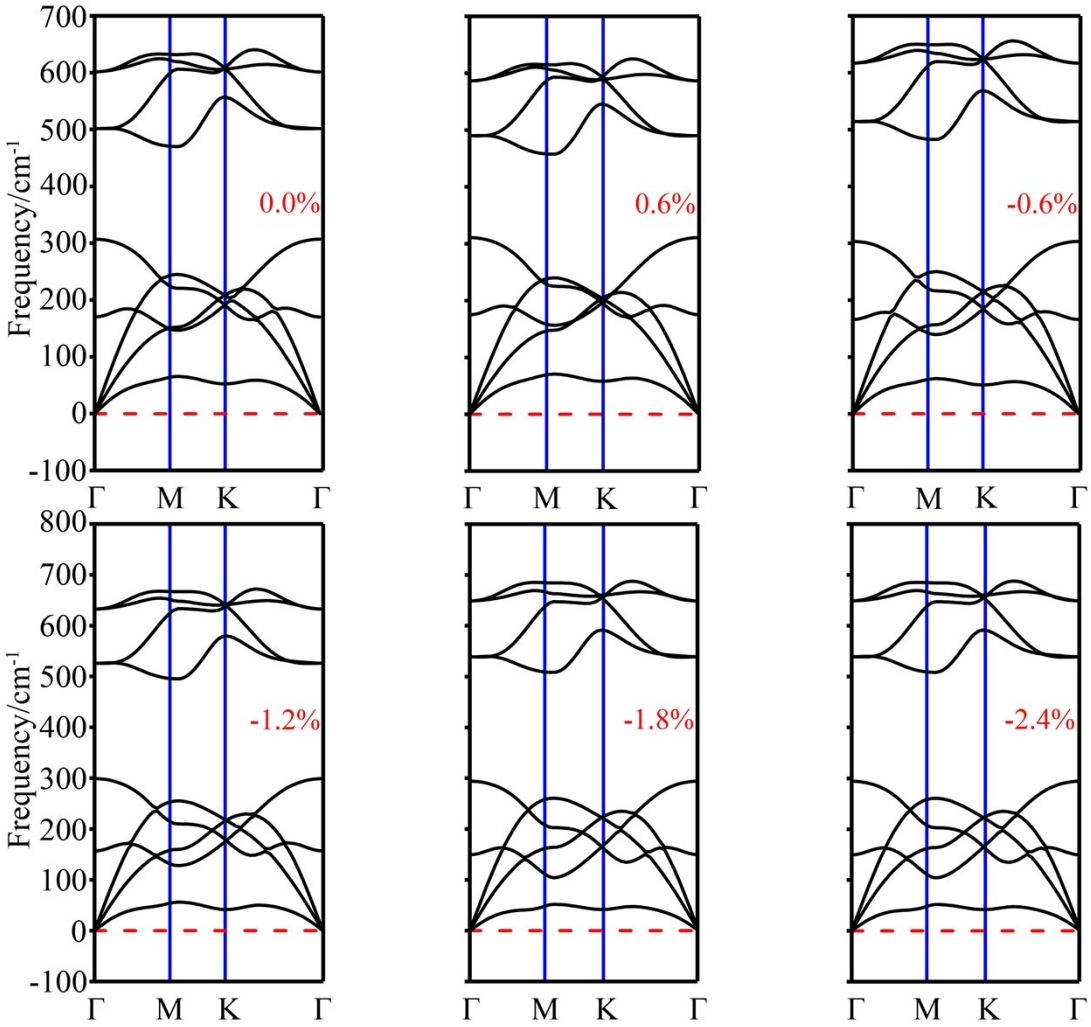

Figure S6. Phonon dispersion spectra of Be_2Ga under strain from -2.4% to 0.6%.

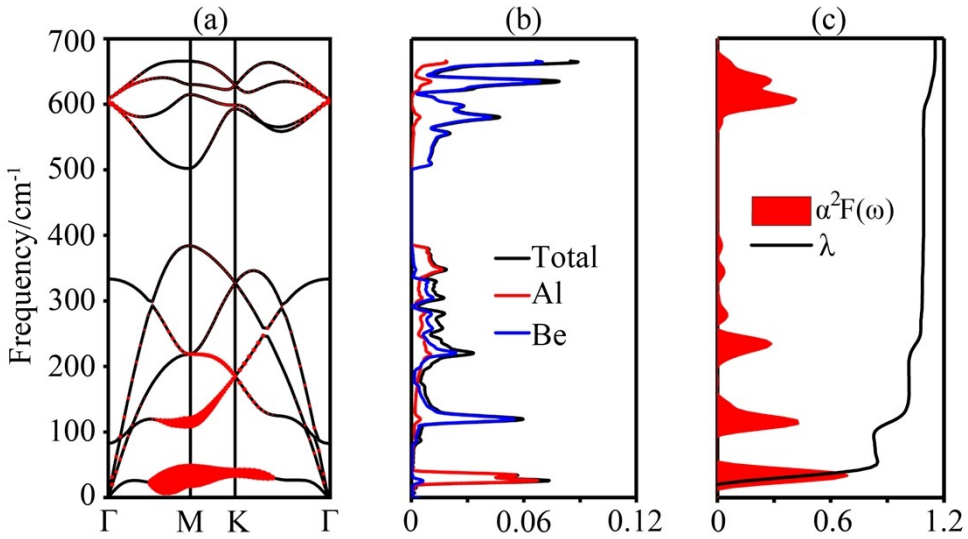

Figure S7. (a) Phonon dispersion with electron-phonon coupling strength, (b) phonon density of states (PhDOS), (c) Eliashberg spectral function $\alpha^2F(\omega)$ and the overall electron-phonon coupling strength $\lambda(\omega)$ of Be_2Al under the strain of -0.5%.

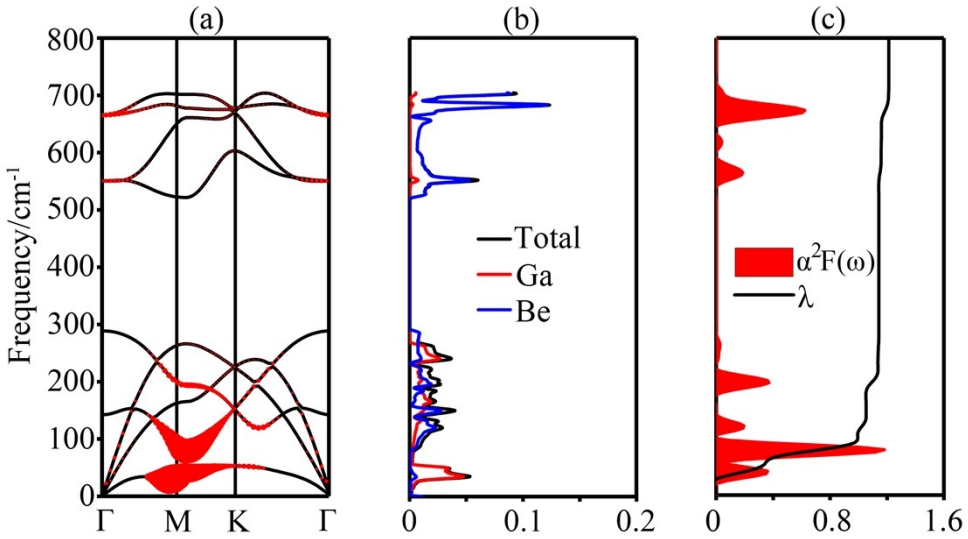

Figure S8. (a) Phonon dispersion with electron-phonon coupling strength, (b) phonon density of states (PhDOS), (c) Eliashberg spectral function $\alpha^2F(\omega)$ and the overall electron-phonon coupling strength $\lambda(\omega)$ of Be_2Ga under the strain of -2.4%.

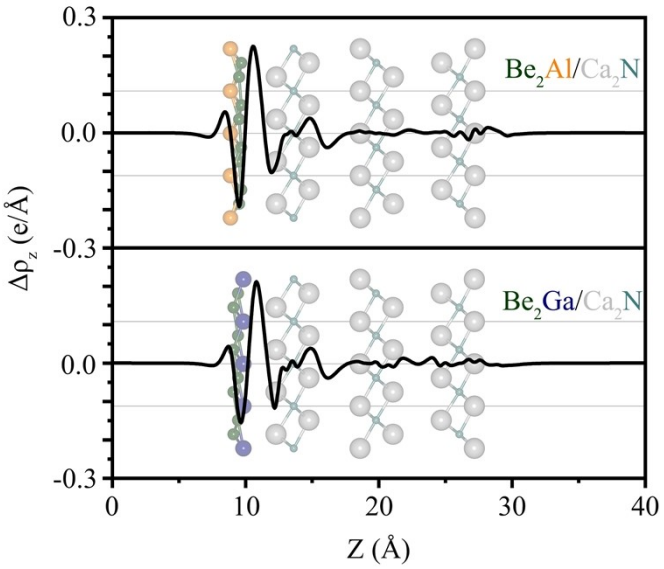

Figure S9. Plane-averaged charge density difference along the vertical z-direction to the Be_2M (M =Al, Ga) monolayer and the Ca_2N substrate.

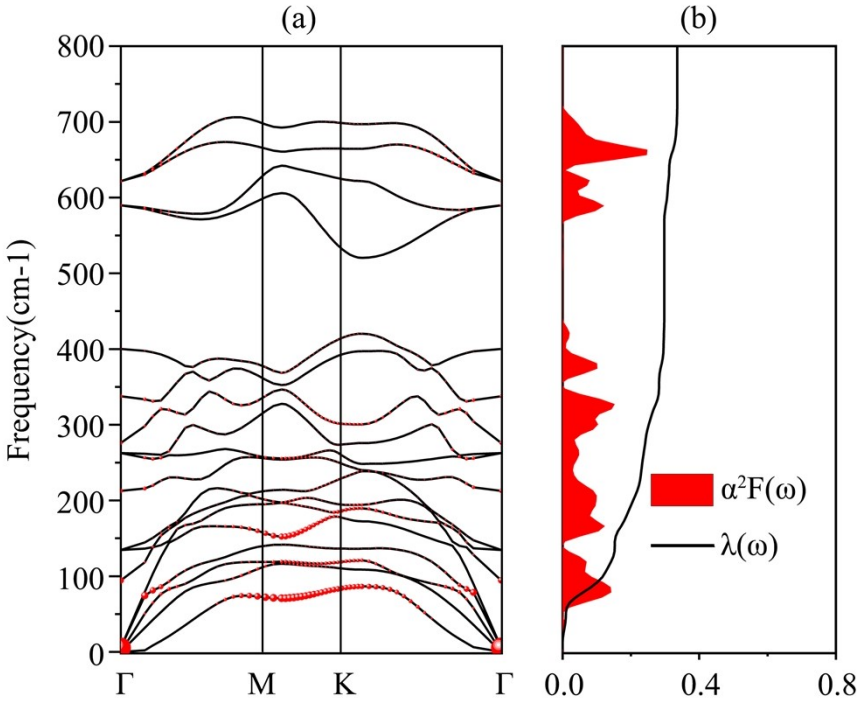

Figure S10. (a) Phonon dispersion with electron-phonon coupling strength, (b) Eliashberg spectral function $\alpha^2F(\omega)$ and the overall electron-phonon coupling strength $\lambda(\omega)$ of the Be_2Al-Ca_2N bilayer.

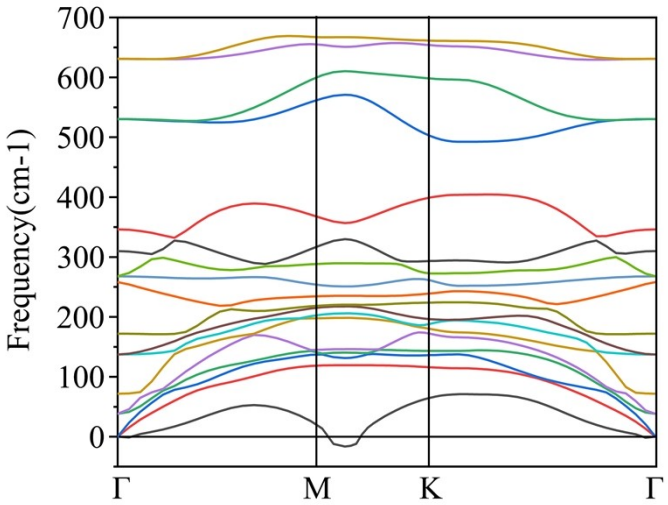

Figure S11. Phonon dispersion of the Be_2Ga-Ca_2N bilayer.