Supporting Information

Structural properties and strain engineering of BeB_2 monolayer from first-principles

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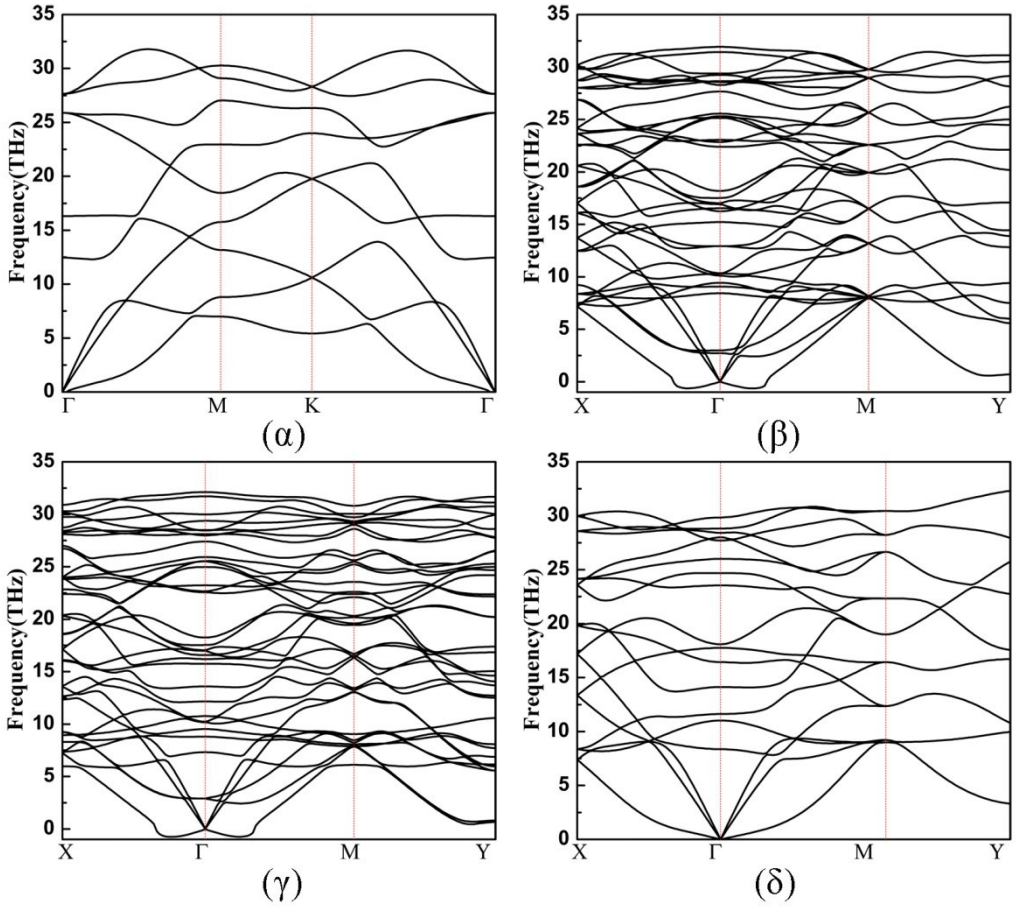
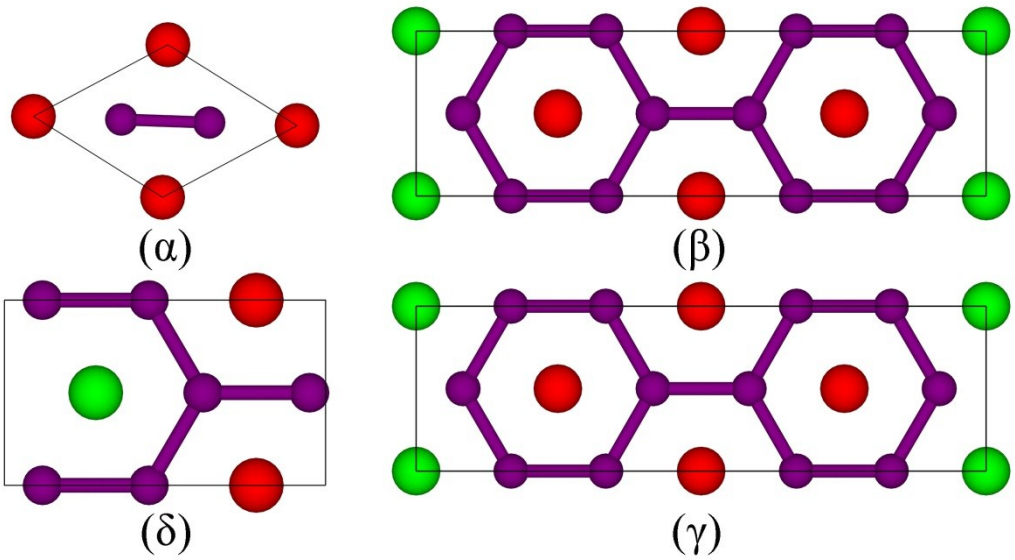


Figure S1. The phonon dispersion curves of the α, β, γ and δ phase BeB_2 monolayer.

Computational details for phonon spectrum

The BeB_2 monolayer was placed in *xy* plane with *z* direction perpendicular to the layer plane and a vacuum slab of 20 Å in *z* direction is included. The unit cells of α, β, γ, δ phases for phonon spectrum calculations are displayed in Figure S2. The red spheres represent Be atoms located below B sheet, while the green spheres represent Be atoms above B sheet. The unit cells of α contains 3 atoms, δ phases contain 6 atoms, whereas β and γ phases contain 12 atoms.



FigureS2. The unit cells of α, β, γ, δ phase BeB_2 monolayers for phonon spectrum calculations.

Phonon dispersion analysis was performed by using the Phonopy code implemented with the density functional perturbation theory (DFPT). The energy cutoff was chosen to be 400 eV. The smearing width of 0.1eV based on the Methfessel-Paxton method was performed. For α phase, the supercell contains 5×5×1 unit cells (25 Be atoms and 50 B atoms), the k-point mesh was 12×12×1, the energy and force precision was set to 10^{-6} eV and 5×10^{-3} eV/Å respectively. For β phase, the supercell contains 3×2×1 unit cells (24 Be atoms and 48 B atoms), the k-point mesh was 12×8×1, the energy and force precision was set to 10^{-6} eV and 1×10^{-3} eV/Å respectively. For γ phase, the supercell contains 3×2×1 unit cells (24 Be atoms and 48 B atoms), the k-point mesh was 8×6×1, the energy and force precision was set to 10^{-6} eV and 1×10^{-3} eV/Å respectively. For δ phase, the supercell contains 4×4×1 unit cells (32 Be atoms and 64 B atoms), the k-point mesh was 10×10×1, the energy and force precision was set to 10^{-7} eV and 1×10^{-3} eV/Å respectively.