Supplementary information

Two dimensional honeycomb-kagome Be_3Pb_2: a mechanically flexible topological insulator with high intrinsic carrier mobilities

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S1. Molecular dynamics (MD) simulation

To verify the thermodynamic stability of 2D Be_3Pb_2, we carried out a canonical MD simulation by using SIESTA. The exchange and correlation interaction between electrons were described by generalized gradient approximation as parameterized by Perdew, Burke, and Ernzerhof; while the interaction between electrons and ions was modeled by the norm-conserving pseudopotential. The energy cutoff was as high as 200 Ry. The structure employed in MD simulation is a rectangular shaped supercell of 2D Be_3Pb_2 with a size of 40.95×42.56 $Å^2$. The temperature was set to be 300 K, and the time step 1 fs. The snapshot of the structure after 5 ps is shown in Fig. S1. Apparently, we do not spot any broken bonds between Be and Pb atoms. Hence, the 2D Be_3Pb_2 is thermodynamically stable at room temperature.

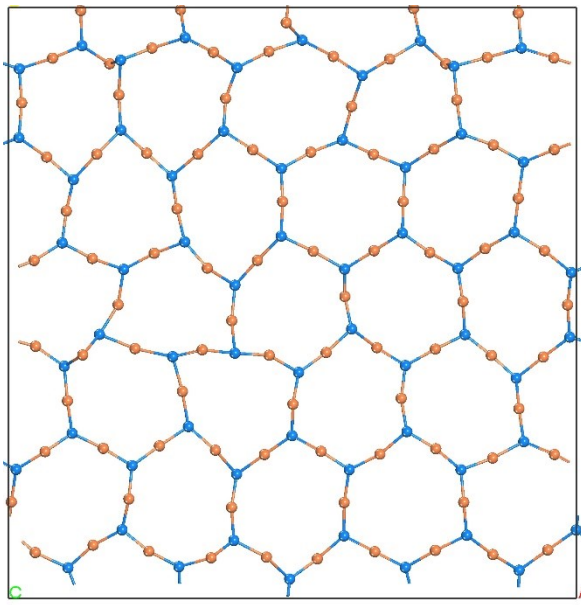

Figure S1. A snapshot of 2D Be3Pb2 after a canonical molecular dynamics simulation.

S2. Phonon dispersion

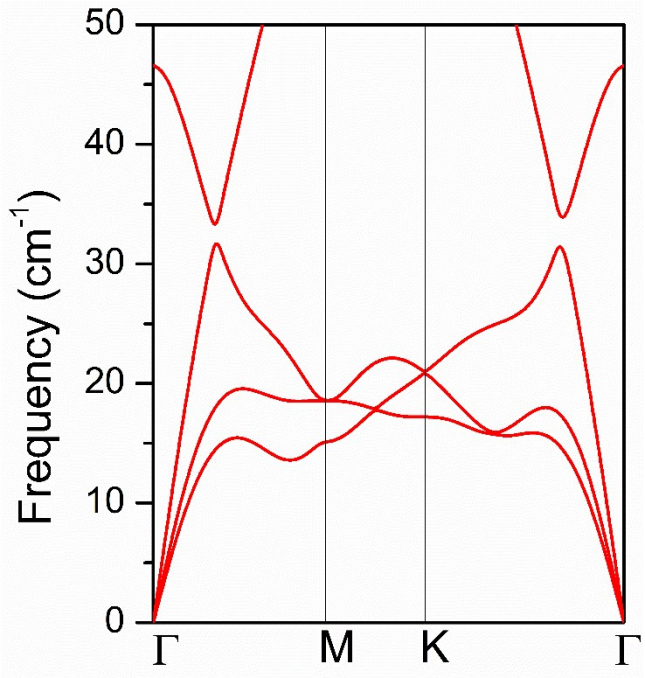

Figure S2. Dispersions of acoustic phonons.

S3. Deformation potential

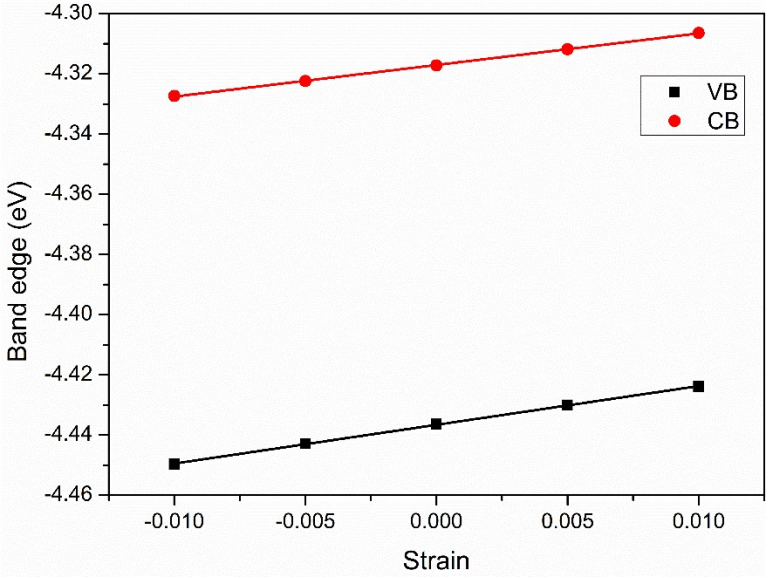

Figure S3. The band edges as a function of mono-axial strain exerted along the zigzag

direction. The energies of band edges are referenced to the vacuum level. The slopes of linear fitting curves give rise to the deformation potential constants for both valence (VB) and conduction (CB) bands.

S4. Band structures of strained 2D Be3Pb2.

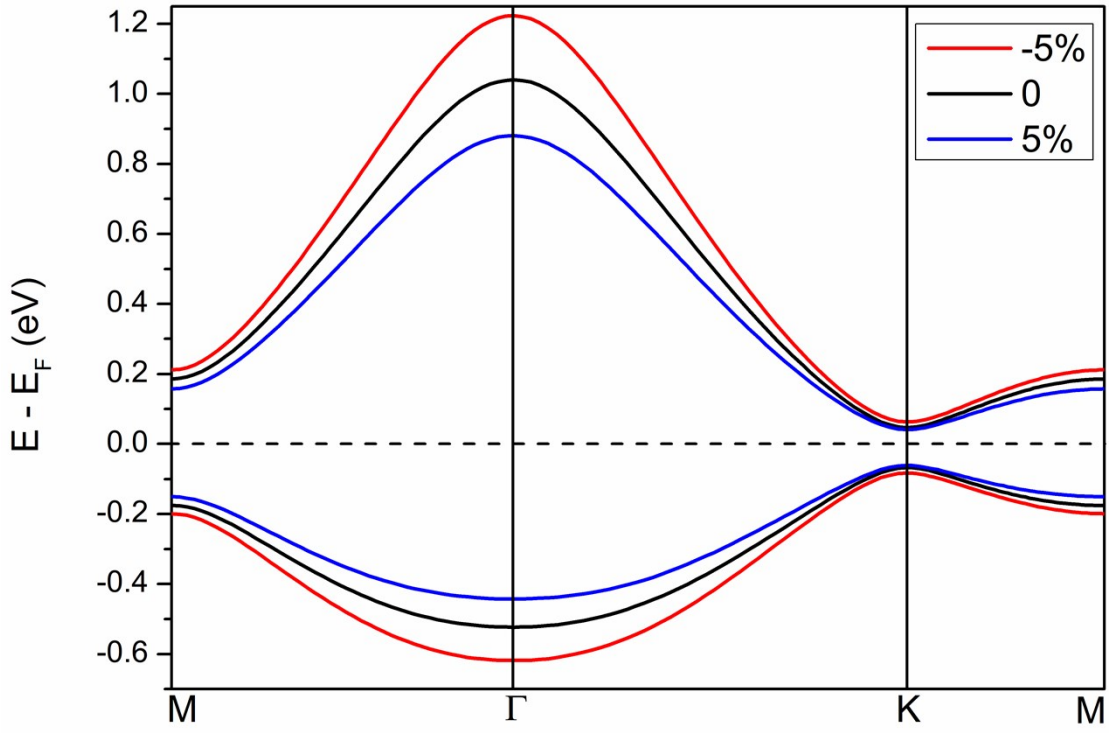

Figure S4. The lowest conduction bands and highest conduction bands of the biaxial-strained 2D Be_3Pb_2.