Supplemental Materials

Two-dimensional Honeycomb B$_2$Se with Orthogonal Lattice: High Stability and Strong Anisotropic Dirac Cone

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Figure S1. (a) The phonon spectrum of enlarged view of the range of 0-100 cm\(^{-1}\) for \(c\)-B\(_2\)Se. (b) The phonon spectrum of enlarged view of the range of 0-100 cm\(^{-1}\) for \(p\)-B\(_2\)Se.

Figure S2. (a) Variations of the total potential energy up to 10000 fs during \textit{ab initio} molecular dynamics (AIMD) simulations at 700 K for \(c\)-B\(_2\)Se. (b) Snapshots of the AIMD simulation for the structure of \(c\)-B\(_2\)Se at times of 10000fs.
Figure S3. (a) and (b) Top views of c-B$_2$Se and p-B$_2$Se. The unit cell are marked with a dotted line. B$_1$ and B$_2$ represent the boron atom with different chemical environments.

Figure S4. Band structures of c-B$_2$Se under different intensity of the spin orbit coupling (SOC) effects with corresponding $\lambda$ marks in each band diagram.
Figure S5. (a) The total energy of \( c{-}B_2Se \) under uniaxial strain as a function of the strain along \( a \) and \( b \) directions, respectively. The in-plane stiffness \( C \) can be obtained by fitting the parabola. (b) The position of Fermi level with respect to lattice compression and dilation. The slope of the straight lines gives the deformation potential (DP) constant.

Figure S6. Band structures of \( p{-}B_2Se \) under different intensity of the SOC effects with corresponding \( \lambda \) marks in each band diagram.

Figure S7. (a) The total energy of \( p{-}B_2Se \) under uniaxial strain as a function of the strain along \( a \) and \( b \)
We apply a 2% uniaxial strain ($\delta$) to the material and observe the change in total energy, as shown in Fig. S5 (a) and Fig. S7 (a). According to the formula
\[ \frac{\Delta E}{S_0} = \left( \frac{C}{2} \right) \times \left[ \frac{(a - a_0)}{a_0} \right]^2, \]
where $S_0$ is the area of the optimized cell, $\Delta E$ is the energy difference, quadratic fitting the parabola can get $C$, as shown in Fig. S5 (a) and Fig. S7 (a). Considering the especial band structure of the Dirac cone, we use the change of the Fermi level as a function of uniaxial strain. The relationship between the Fermi level position and $\delta$ are shown in Fig. S5 (b) and Fig. S7 (b). The slope of the line corresponds to the DP constant in different directions.