## **Support Information**

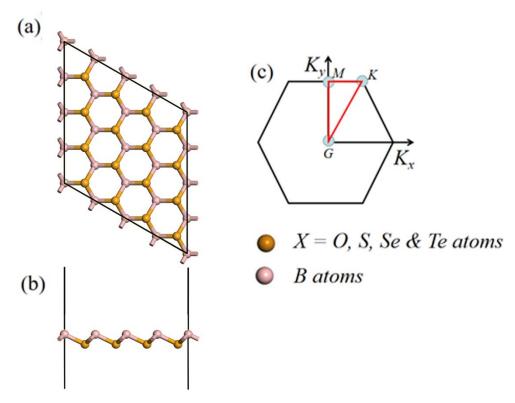


Fig. S1 (a) and (b) Top view and side view of monoatomic-layer hexagonal BX (X = O, S, Se, and Te). (c) Brillouin zone of monolayers H- and F-BX (X = O, S, Se, and Te) with high-symmetry points.

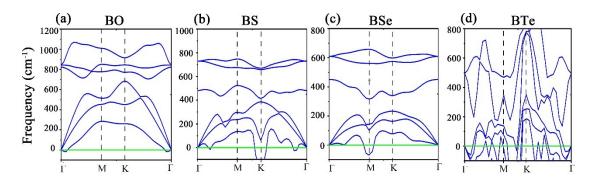


Fig. S2 (a)-(d) the phonon spectra of monoatomic-layer hexagonal BX (X = O, S, Se, and Te).

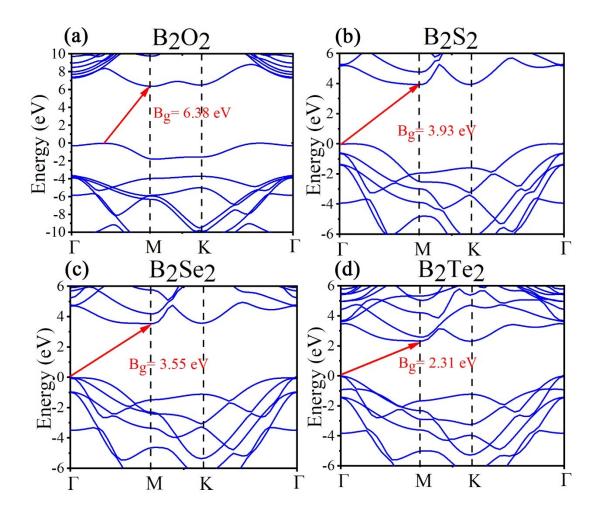


Fig. S3 (a)-(d) Band structures of 1T monolayers  $B_2X_2$  (X = O, S, Se, and Te).