Supplementary Information

One Dimensional Nearly Free Electron States in Borophene

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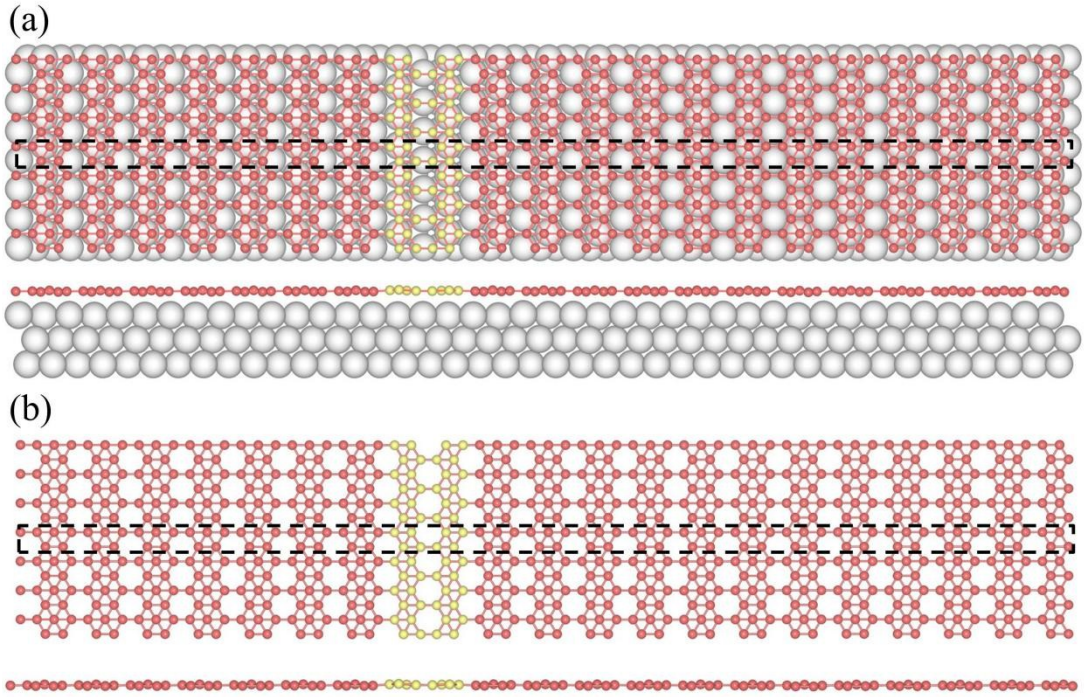

Figure S1. Top and side views of intermixing borophene (a) with Ag(111) substrate and (b) without substrate. Red and gray balls represent boron and silver atoms, respectively. The yellow balls is the line defect. The black dashed line indicate the superlattice used in calculations.

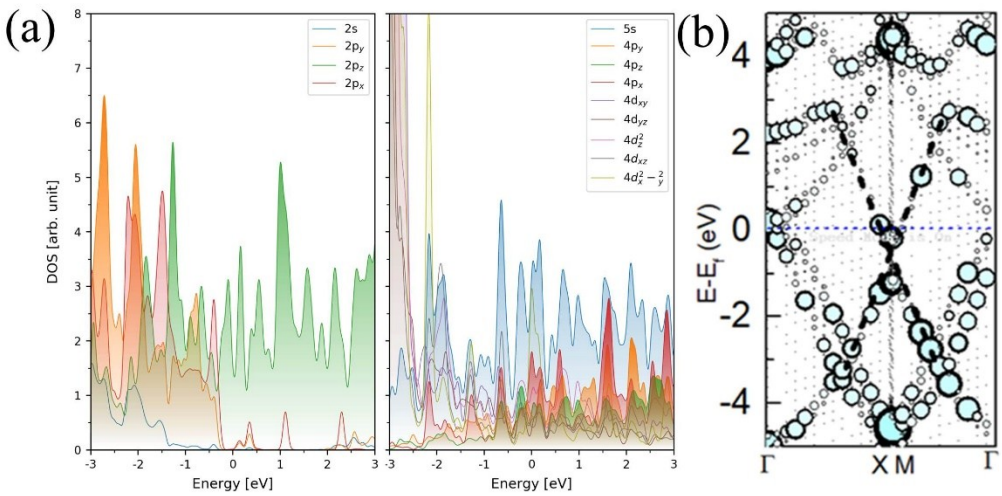

Figure S2 (a) Orbital resolved partial density of states of boron and silver atoms in the borophene/Ag(111) system. (b) Unfolded bands of borophene containing line defects, the black line intersection indicates the Dirac cone.

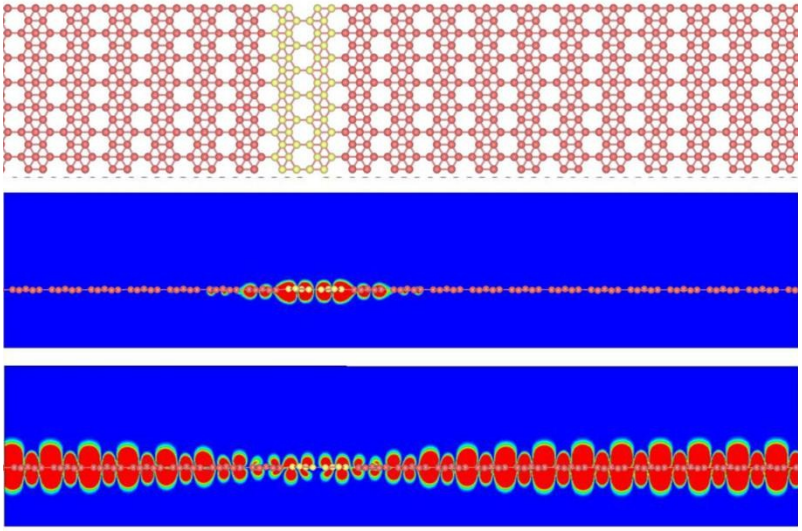

Figure S3. The real-space distribution of partial charge density for π* states. The top panel is the atomic structure of freestanding borophene with linear defect. The middle and bottom panels present two unoccupied states below 1st states (see the band structure in Figure 3a) in the main text), which are attributed to normal π* electronic states and therefore do not exhibit delocalized spatial distribution (i.e. NFE features). The side view of freestanding borophene atoms are overplayed on charge density figures to guide eyes.

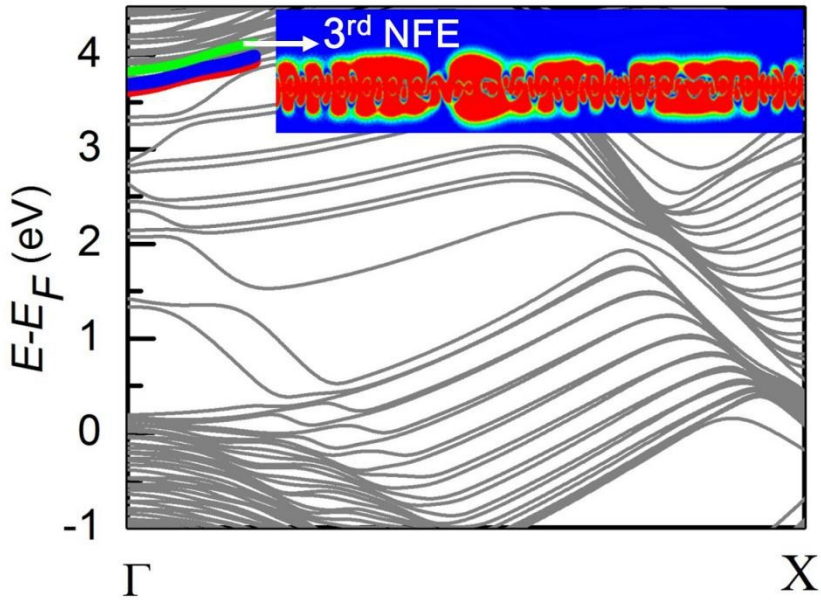

Figure S4. Band structures of freestanding borophene with line defect. The red, blue and green lines represent the 1st, 2nd and 3rd NFE states, respectively. The inset in the topmost part shows the the real-space distribution of partial charge density at Γ point for 3rd NFE states. Figure 3b in the main text shows the real-space distribution of 2nd and 3rd NFE states.

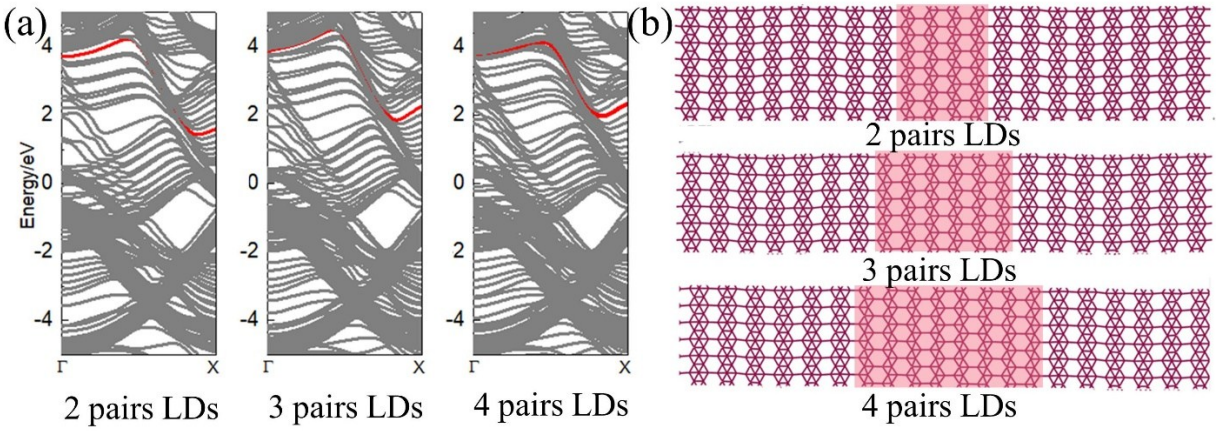

Figure S5. (a) Band structures of monolayer boron with different width of the line defects (LDs). (b) The corresponding optimized structures of β_{12} sheet with different number of χ_3 rows as line defects (pink shaded region).