Electronic Supplementary Information for

Stable and metallic borophene nanoribbons from first-principles calculations

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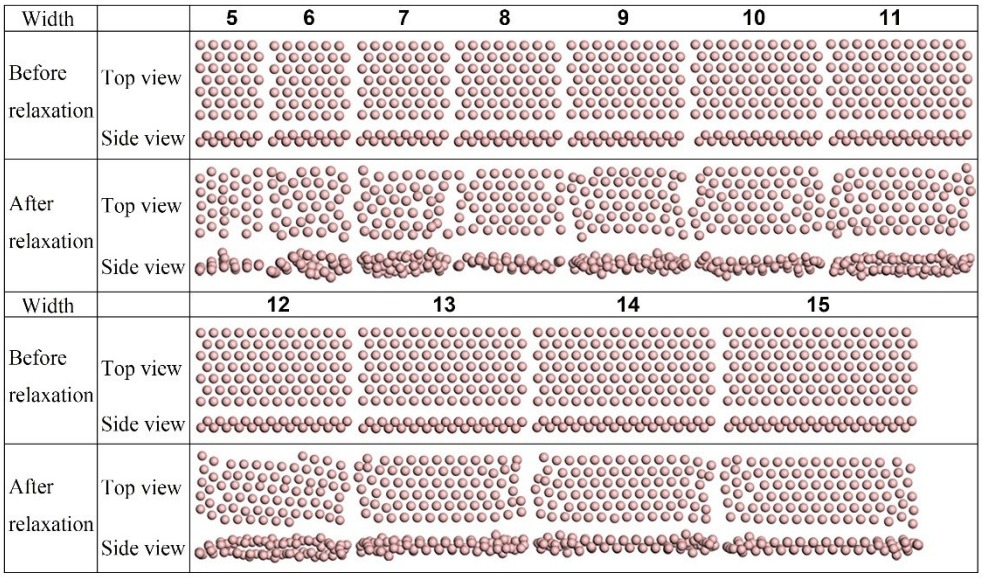

Figure S1. Structural relaxations of the zigzag-edge borophene nanoribbons are shown above. As seen, the nanoribbon structure completely crashes when its width is less than 13. In wider nanoribbons, the edge atoms become disordered.

The structure relaxations of the zigzag-edge boronphene nanoribbons are shown in Figure S1. As this kind of nanoribbon breaks the one-dimensional π system along the boron rows, their edge structures are significantly unstable. As seen above, when the width of nanoribbons is less than 13, the whole structures become crashed. As the width increases to 15, the center atoms are less affected, the edge atoms, however, still become disordered. We, therefore, conclude that the zigzag-edge borophene nanoribbons are not stable. In the manuscript, only the line-edge borophene nanoribbons are discussed.

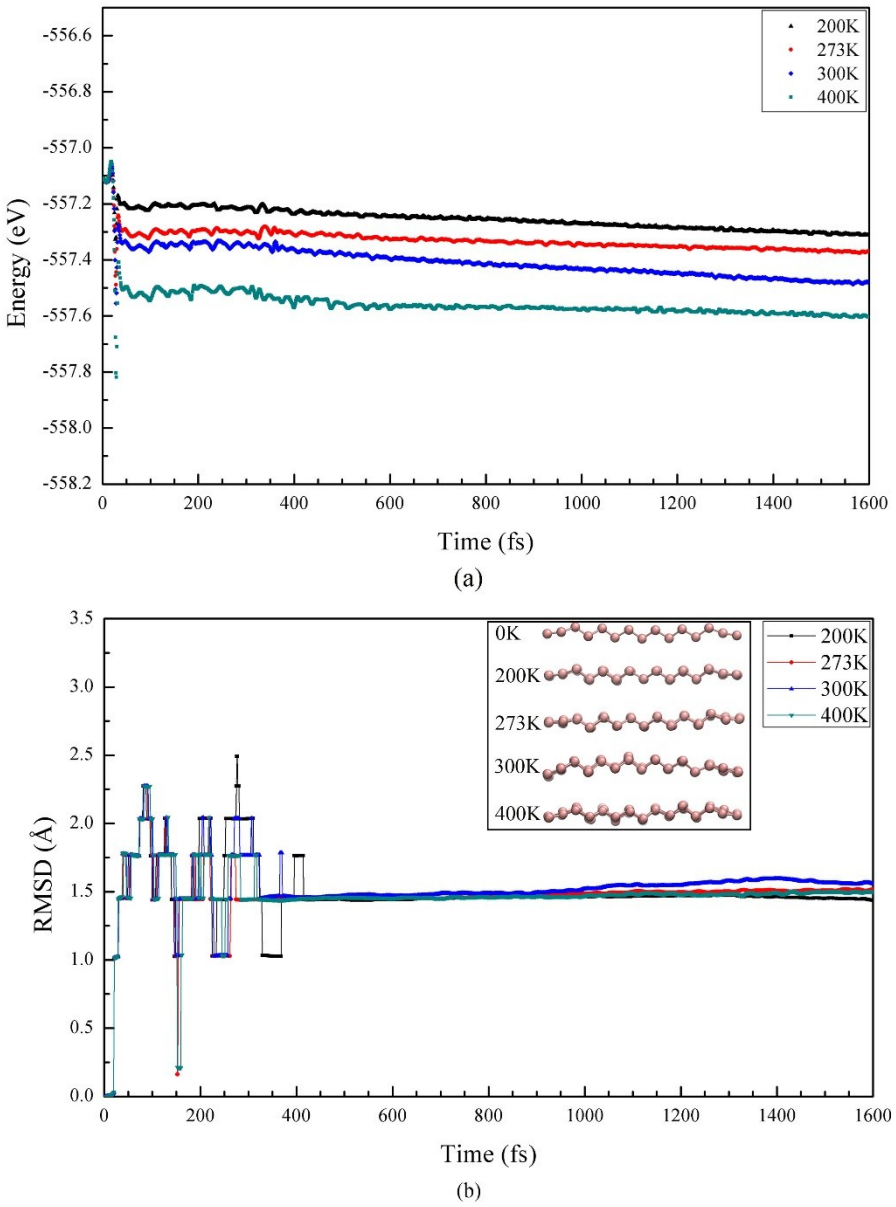

Figure S2. The molecular dynamic simulation analysis of the 15-atom-width line-edge borophene nanoribbon (15 BNR) in (a) energy and (b) root-mean-square deviation (RMSD) at 200 K (black), 273K (red), 300 K (blue) and 400 K (dark cyan). The insets of (b) are the atomistic structures of 15 BNR after 1600fs at different temperatures.

Figure S2 shows the molecular dynamic calculations for 15 BNR at 200 K, 273K, 300 K and 400 K. The corresponding plots of energy and RMSD with respect to the

simulation time show that the curves reaches stable equilibrium after about 500 femtoseconds. As the maximum RMSD of 15 BNR is only 2.491 Å in the MD simulations, the atomic structures should not differ too much from their initial positions. This is confirmed by the atomistic structures shown in the inset of Fig. S2 (b). As a consequence, we predict that the borophene nanoribbons are stable in their free-standing form.

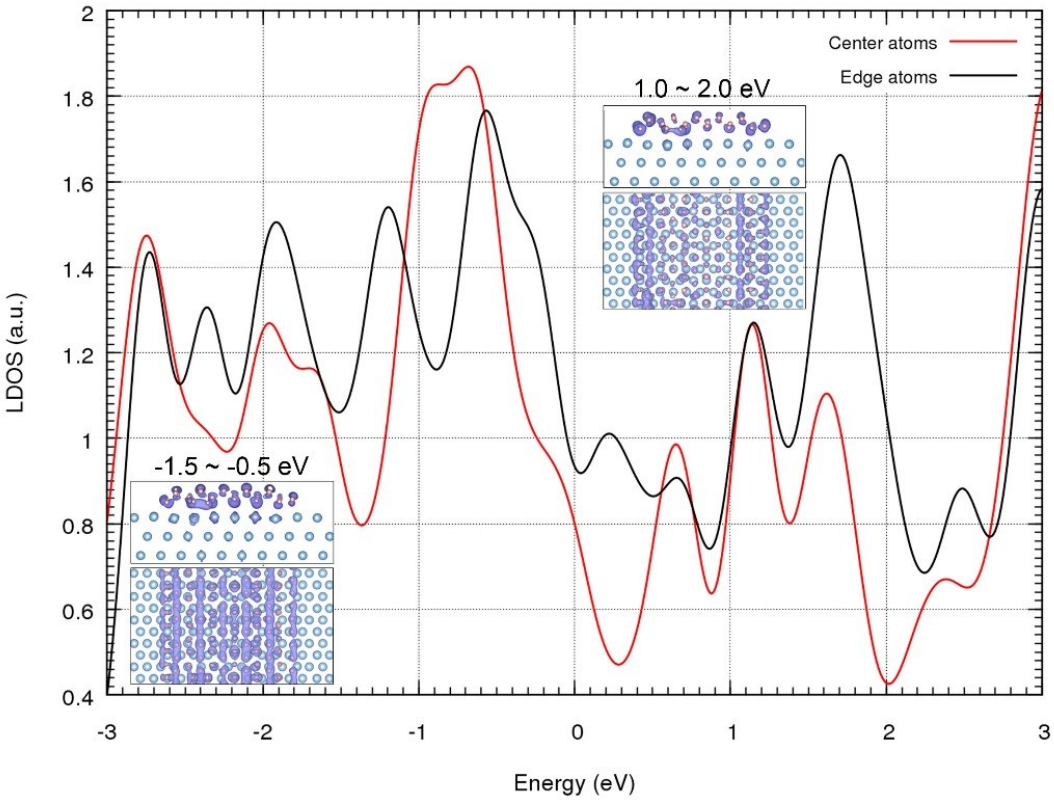

Figure S3. The Local Density of States (LDOS) of a 12-atom-width line-edge borophene nanoribbon adsorbed on an Ag (111) surface**.** The LDOS of the center and edge boron atoms are shown by red and black solid curves, respectively. The insets are the band decomposed charge distributions at [-1.5,-0.5] and [1.0, 2.0] eV. The isosurface value is 0.007 e/Å^3.

The PDOS plot of a 12-atom-width line-edge borophene nanoribbon (BNR) adsorbed on an Ag surface is shown in Fig. S3. As seen, the states of BNR near fermi are significantly increased (Fig. 4 and Fig. S3), due to the interaction between the adsorbate and substrate. Correspondingly, the occupied states of adsorbed BNR are dramatically hybridised, while the population difference of the empty states between the centre atoms and edge atoms are reduced.