Supporting Information

The direct-current and alternating-current transport properties of bilayer α- and α†-borophenes

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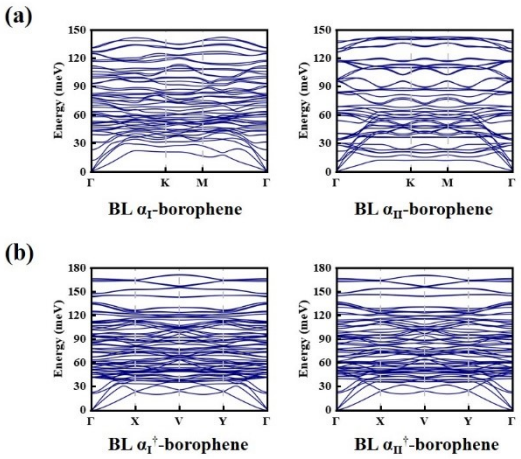

Fig. S1. The phononic energy bands of (a) BL α_I- and α_{II}-borophenes and (b) BL $\alpha_I^\dagger$- and $\alpha_{II}^\dagger$-borophenes.

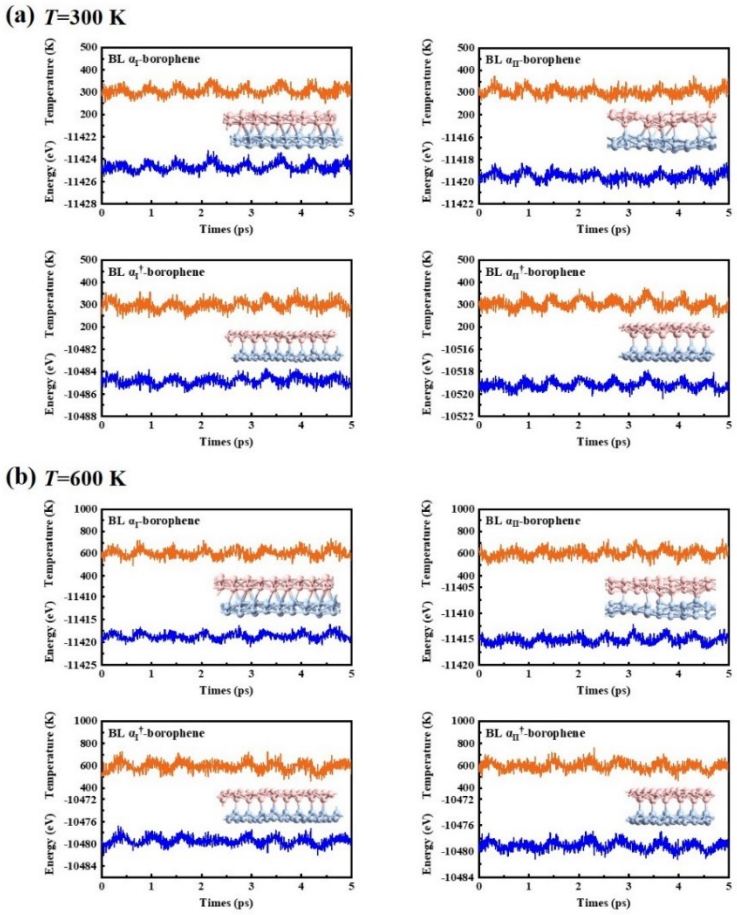

Fig. S2 The fluctuations of temperature and total energy with time for BL α_I-, α_{II}-, $\alpha_I^\dagger$- and $\alpha_{II}^\dagger$-borophenes at (a) 300 K and (b) 600 K. The inset shows the corresponding structure after 5000 time steps.

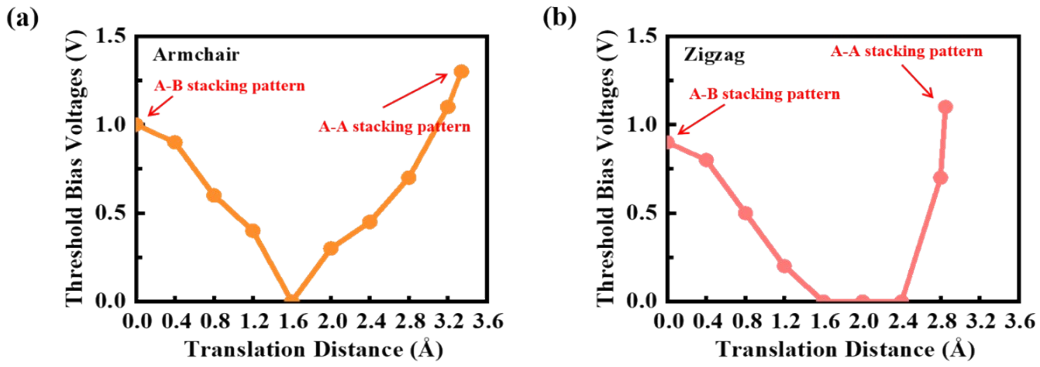

Fig. S3 The threshold bias voltages of BL α†-borophene for the top layer translation along the (a) armchair and (b) zigzag directions.

There are many stacking patterns for BL α†-borophene. Here, we considered two typical cases, *i.e.* the top layer translates along the armchair or zigzag direction while the bottom layer keeps still (the translational distance is 0.4 Å). The calculated threshold bias voltages of these different stacking patterns are given in Fig. S3. We found that the threshold bias voltage gradually decreases and changes to zero (these stacking patterns have metallic characteristics), and then gradually increases. Nevertheless, near the considered A-B or A-A stacking pattern the semiconducting characteristic of BL α†-borophene is still robust for relatively large translational distances.

The appearance of metallic characteristics is easy to understand. Compared with A-B or A-A stacking pattern, for some given stacking patterns, their translational distances are very large, thus the destruction of the interlayer covalent bonds will release more electrons. In a word, the influences of the stacking patterns on the threshold bias voltages are complicated.

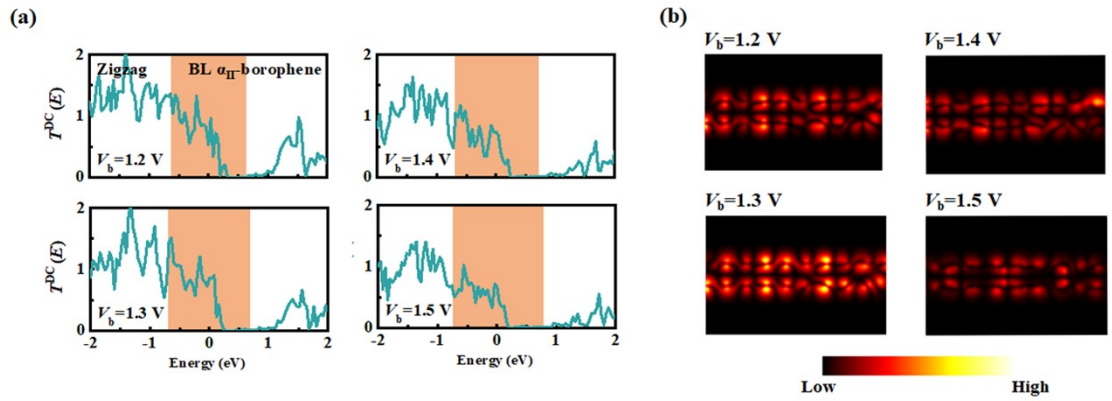

Fig. S4 (a) The DC transmission spectra and (b) the transmission eigenstates at the Fermi level of BL α_{II}-borophene along the zigzag direction. The orange shadow area represents the bias window.

In the bias windows DC transmission spectra become lower when V_b gradually increases and, meanwhile, the related transmission eigenstates exhibit relatively localized behaviors. This means that the transmission probabilities of the electrons become smaller, finally leading to the appearance of the NDR effect along the zigzag direction when V_b>1.1 V.

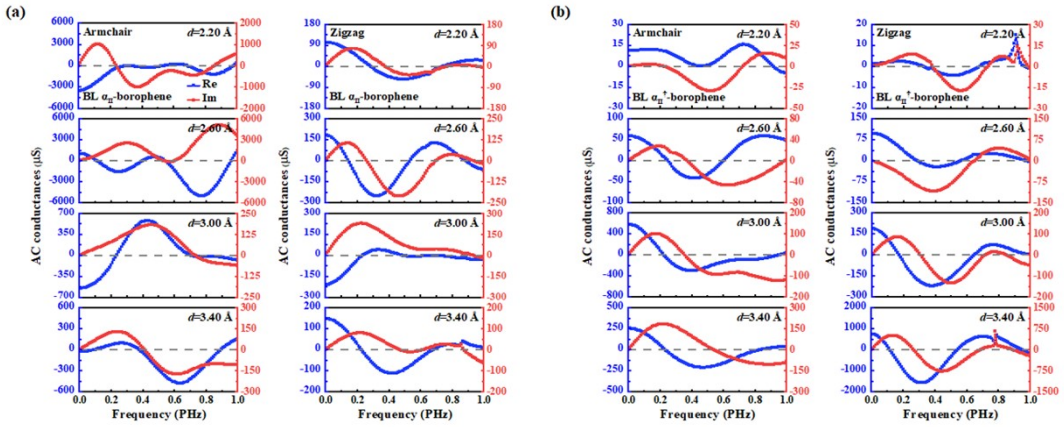

Fig. S5 The AC conductances of BL (a) α_{II}- and (b) $\alpha_{II}^{\dagger}$-borophenes with different interlayer distances.