Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information:

Borophosphene as a promising Dirac anode with large capacity and high-rate capability for sodium-ion batteries

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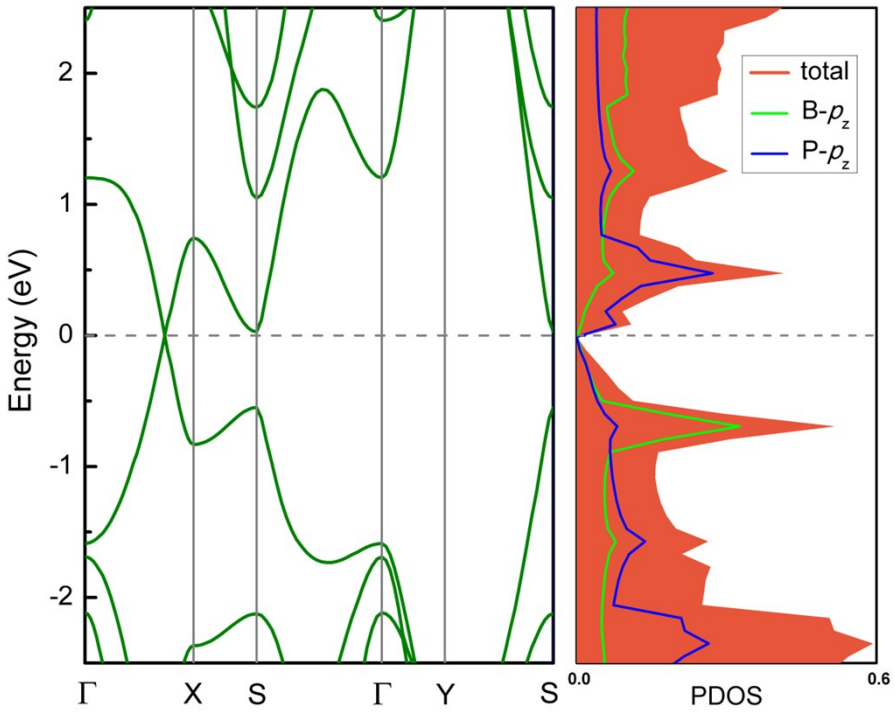

Fig. S1 Calculated band structure and partial density of states (PDOS) of borophosphene. Dash line denotes the Fermi level.

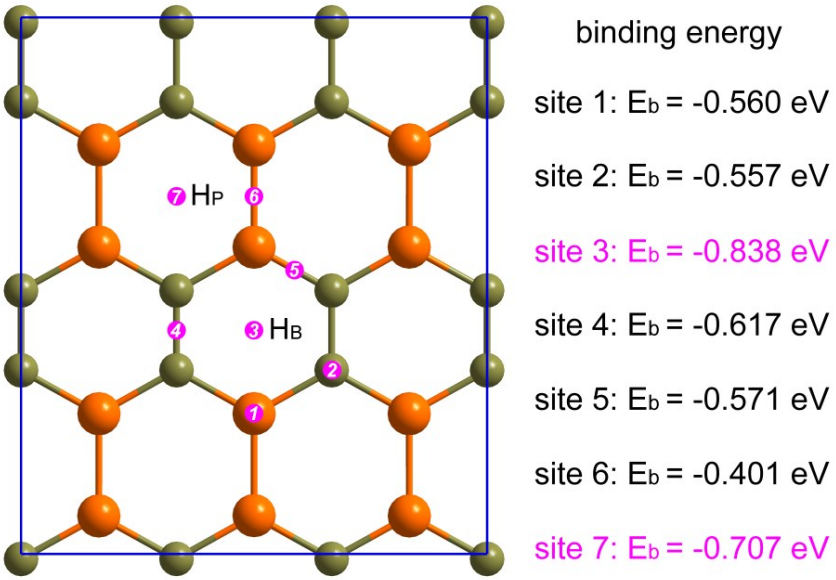

Fig. S2 Schematic diagram for Na adsorption on borophosphene surface. Binding energy at different adsorption sites are shown in right panel. Dark yellow and orange balls denote B and P atoms.

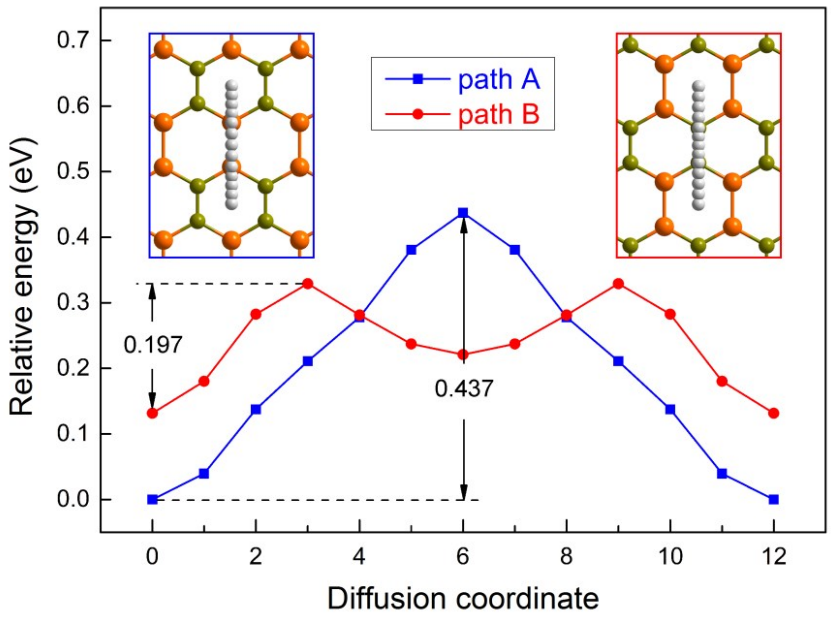

Fig. S3 Diffusion energy barrier of Na atom migrating parallel to B-B or P-P dimer direction. Inserts display the corresponding diffusion pathways: path A (left) and path B (right).

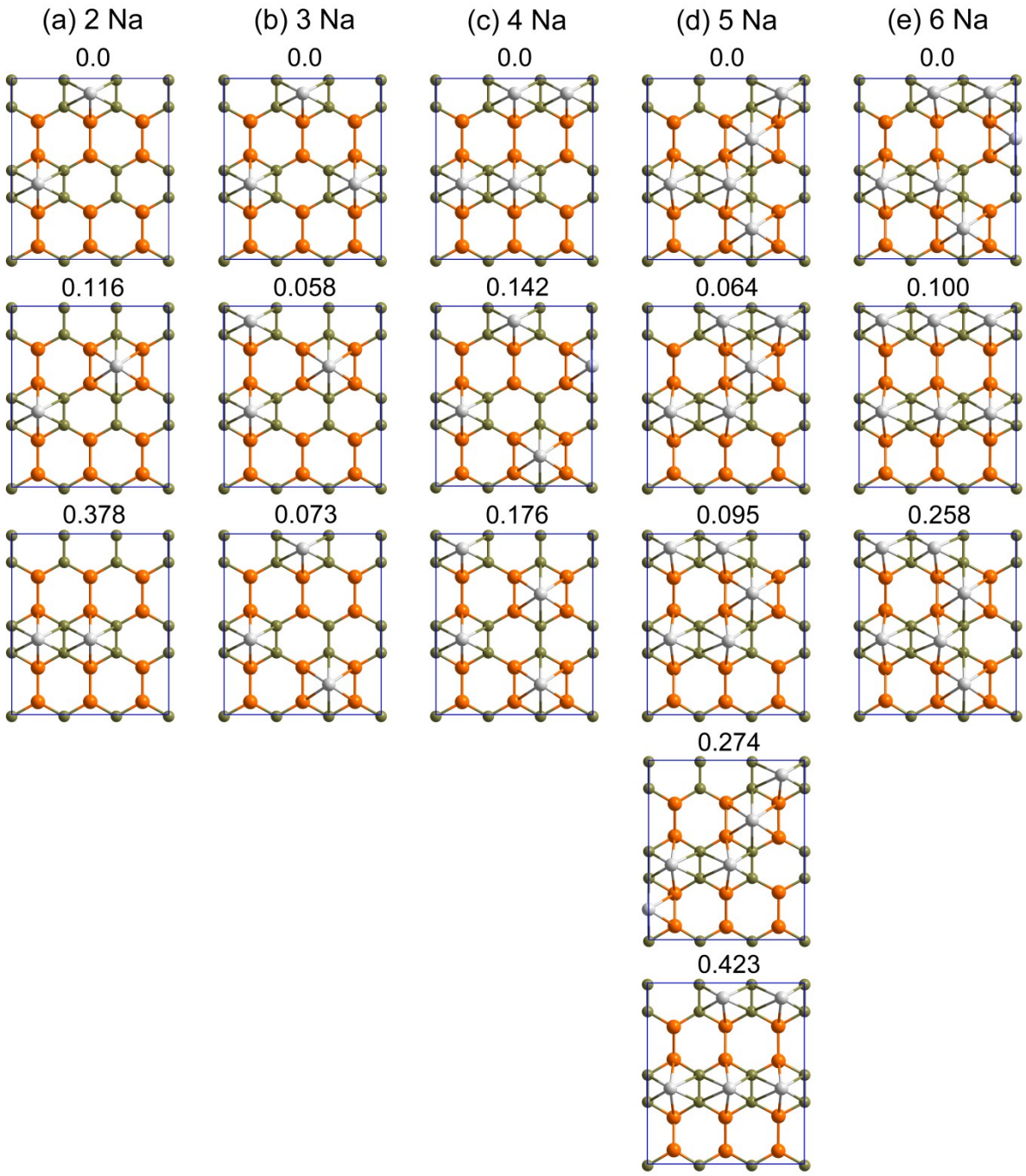

Fig. S4 Various adsorption configurations with relative total energy for Na_xBP species at different Na contents: (a) x = 0.167, (b) x = 0.25, (c) x = 0.333, (d) x = 0.417 and (e) x = 0.5. Dark yellow, orange and gray balls denote B, P and Na atoms, respectively.

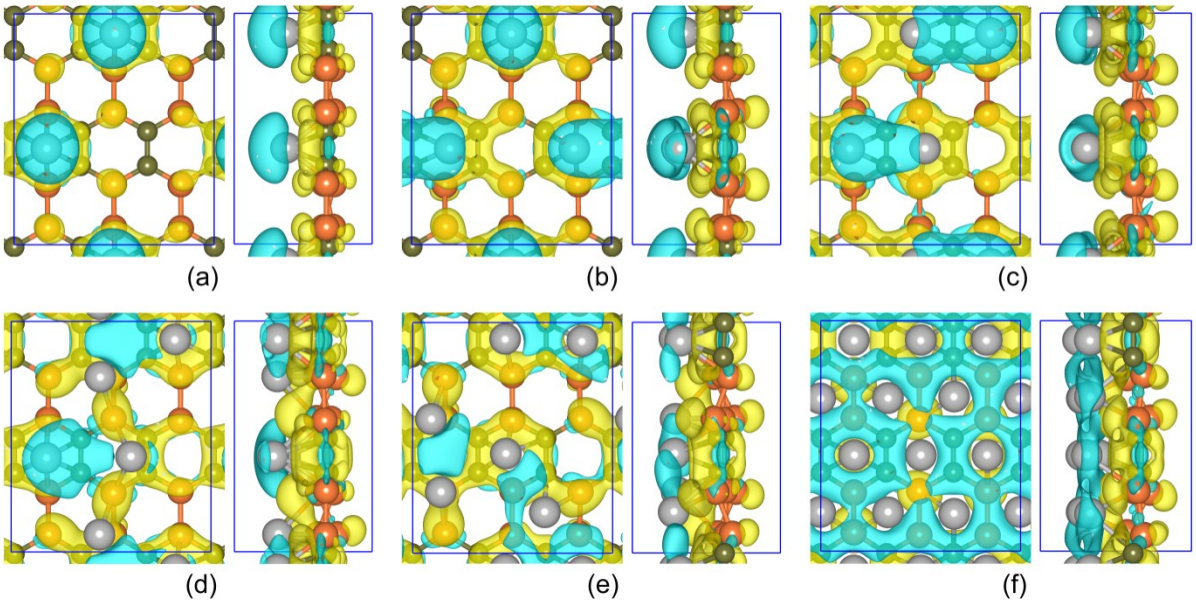

Fig. S5 Difference of charge density of Na_xBP species with different Na contents: (a) x = 0.167, (b) x = 0.25, (c) x = 0.333, (d) x = 0.417, (e) x = 0.5 and (f) x = 1.0. Yellow and turquoise isosurfaces represent electron accumulation ($\Delta\rho>0$) and depletion ($\Delta\rho<0$), and the isosurface level is set to 0.004 e/Å^3.

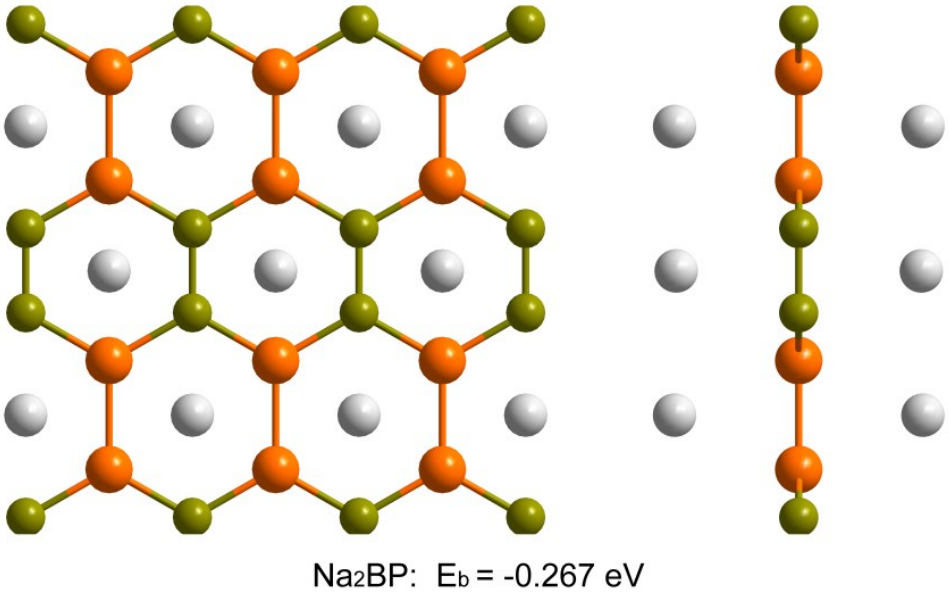

Fig. S6 Optimized adsorption configuration for Na_2BP specie. Its binding energy is -0.267 eV.

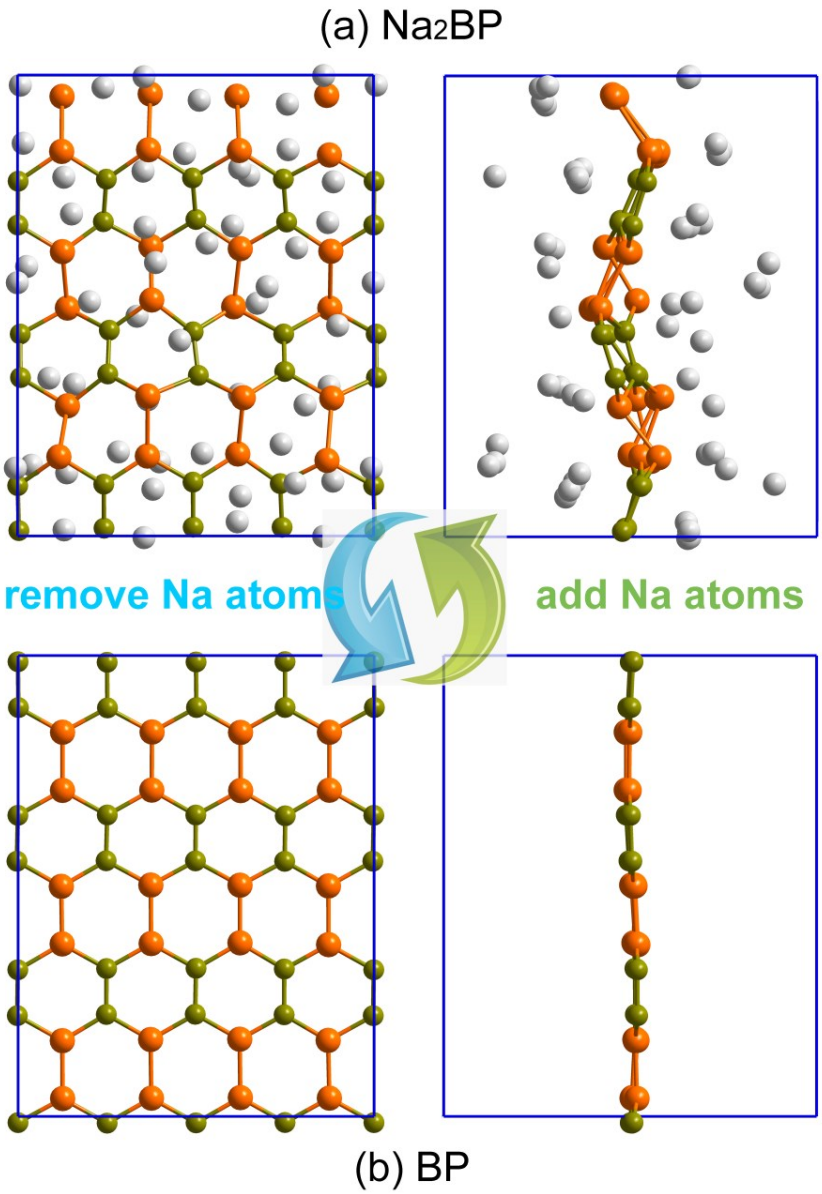

Fig. S7 Snapshots of geometrical configurations after 10 ps AIMD simulation for (a) Na_2BP and (b) the remaining corrugated borophosphene after removing all Na atoms from Na_2BP.

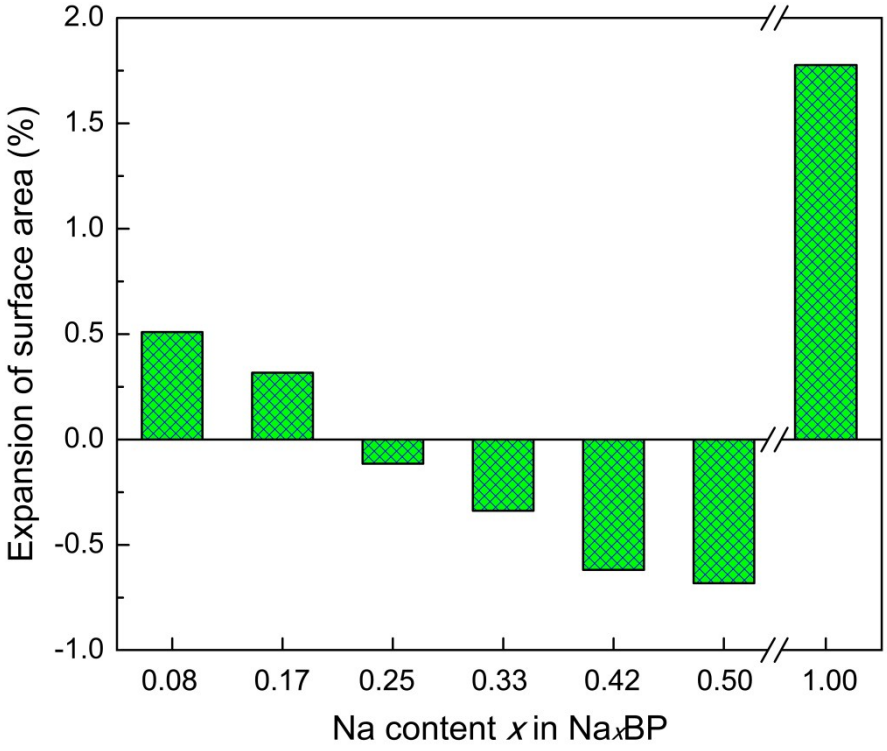

Fig. S8 Expansion of surface area as a functional of Na content x in Na_xBP.