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

Supporting information

BC_2N/Blue Phosphorene Heterostructure as an Anode Material for High-Performance Sodium-Ion Batteries: First Principles Insights

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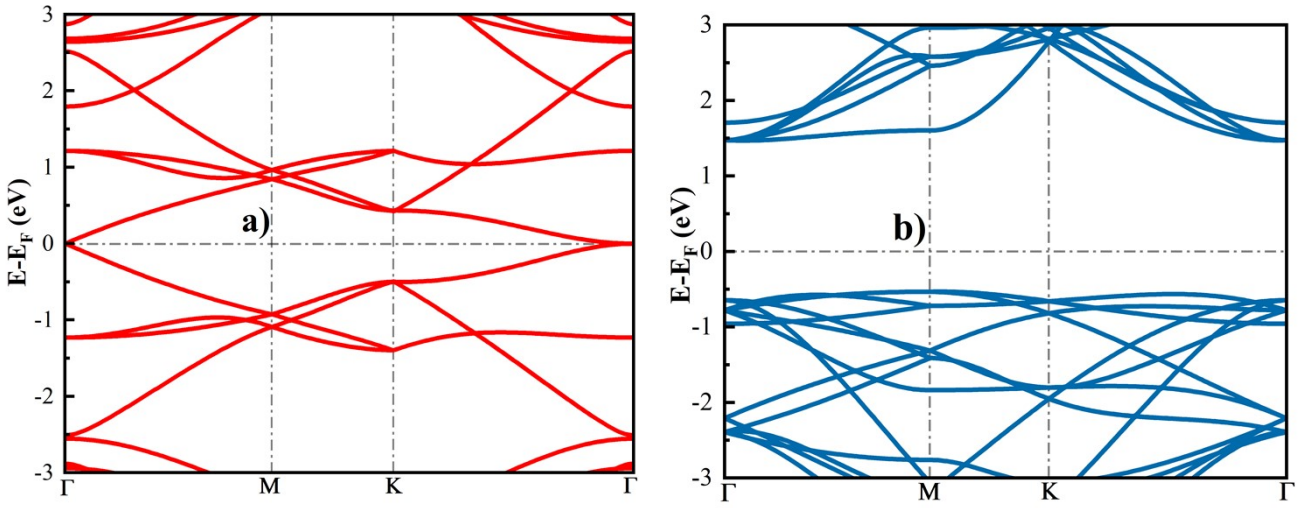

Figure S1. Calculated projected band-structure curves of the (a) pristine BC_2N sheet, (b) pristine Blu-Pn layer. The Fermi energy is set to zero eV, and indicated by a dash-dotted line.

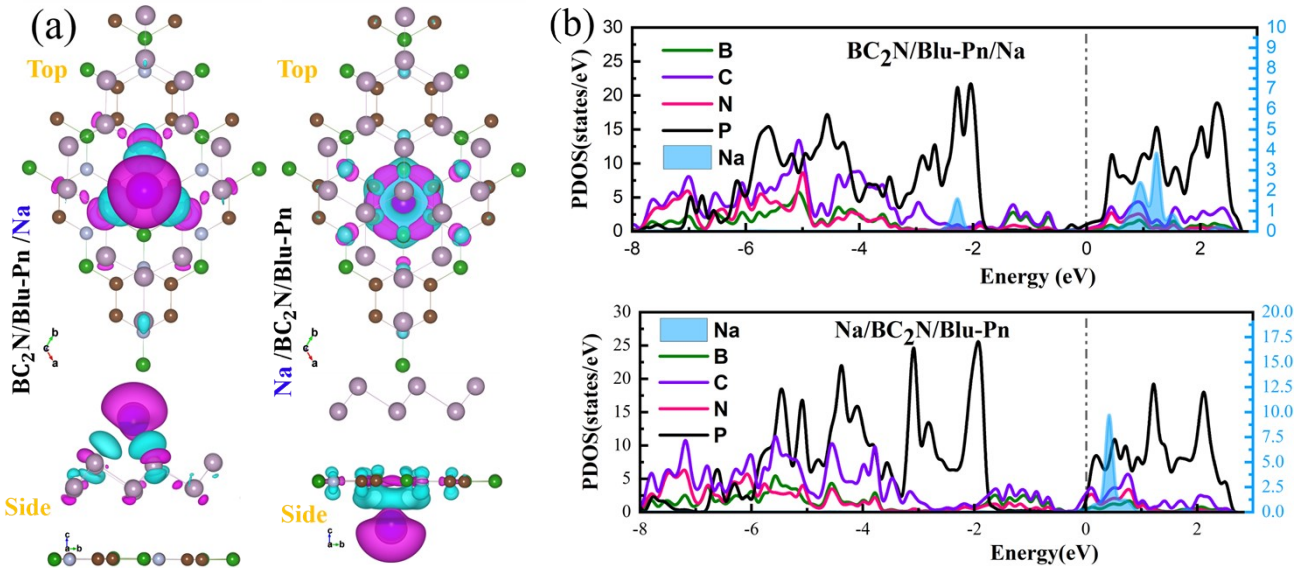

Figure S2. (a) Charge density difference plots of Na adsorption at the most preferable site in the outer-surfaces of Blu-Pn (V_{Pn}-site) and BC_2N (H_{BC}). (b) The Corresponding computed orbital-projected DOS curves. The cyan and magenta colors indicate the charge depletion and accumulation, respectively. The isosurfaces value is taken to be $1.5 \times 10^{-3}\ e/\text{Å}^3$, and the Fermi level is set to 0 eV.