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

Supporting Information for

A first-principle study of BC_3N_2 monolayer and BC_3N_2/graphene heterostructure as promising anode materials for sodium-ion batteries

Xiao-Juan Ye [a], Rui Zhao [b], Xin Xiong [a], Xiao-Han Wang [a], and Chun-Sheng Liu [b*]

[a] College of Integrated Circuit Science and Engineering, Nanjing University of Posts and Telecommunications, Nanjing 210023, China

[b] College of Electronic and Optical Engineering, Nanjing University of Posts and Telecommunications, Nanjing 210023, China

Email: csliu@njupt.edu.cn

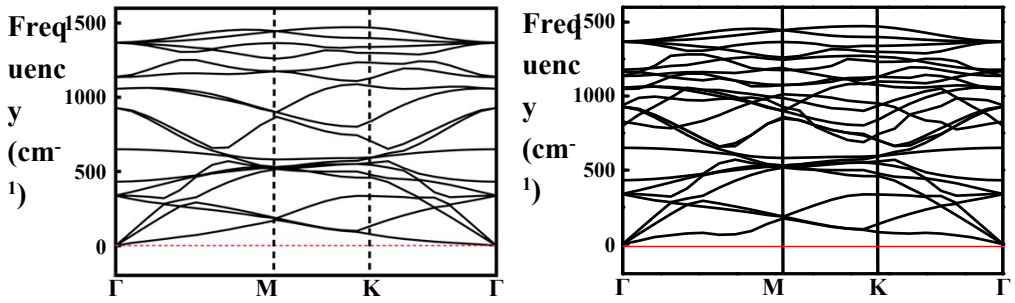

Fig. S1 Phonon dispersion curves of (a) BC_3N_2 monolayer and (b) $Na_2BC_3N_2$.

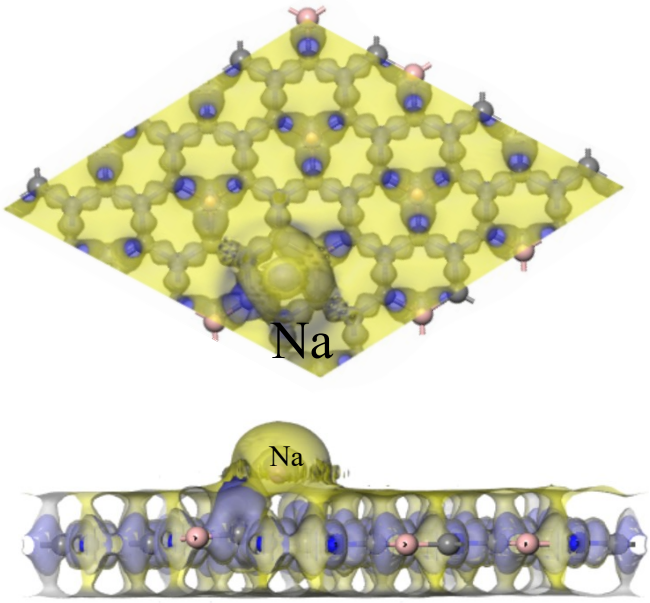

Fig. S2 The top and side view of charge density differences of BC_3N_2 with a Na adsorbed at H site. The iso-surface value is 0.01 eÅ^{-3}, the yellow and blue areas represent the loss and gain of electrons, respectively.

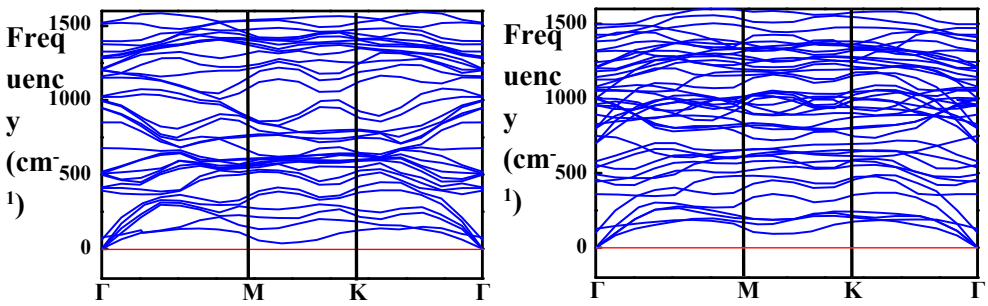

Fig. S3 Phonon dispersion curves of (a) B/G heterostructure (AB stacking) and (b) B/G heterostructure with Na atom adsorbed.

The calculated linear elastic constants (C_{ij}) of BC_3N_2 and B/G heterostructure are shown

in Table S1, which satisfies with the Born criteria ($C_{11} > C_{12}$, $C_{66} > 0$), indicating the mechanical stability of BC_3N_2 and B/G heterostructure with and without Na atoms adsorbed.

Table S1. The calculated linear elastic constants (C_{ij}) of BC_3N_2 monolayer and B/G heterostructure with and without Na atoms adsorbed.

	C_{11} (GPa)	C_{12} (GPa)	C_{66} (GPa)
BC_3N_2	401.2	65.5	167.8
$Na_2BC_3N_2$	398.6	70.8	167.0
B/G	630.4	119.3	284.4
$Na_{3.625}$B/G	625.5	123.6	284.1