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# Two-dimensional $C_3N$/Blue Phosphorene vdW Heterostructure for Li, Na and K-ion batteries.

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## Phonon dispersion spectrum of $C_3N$/BP HS

We have investigated the phonon dispersion spectrum of $C_3N$/BP HS and shown in figure S1. It is always challenging to assess the phonons for heterostructure, which constitute the lattice mismatch. We indeed see some imaginary phonons which are clearly due to the lattice mismatch. However, we must point out that the frequencies of the imaginary modes are small (<100Hz). It may appear as a hindrance to form the heterostructure, however, owing to the low values, the structure can be stabilized by an appropriate substrate, which is typically the case with such systems.

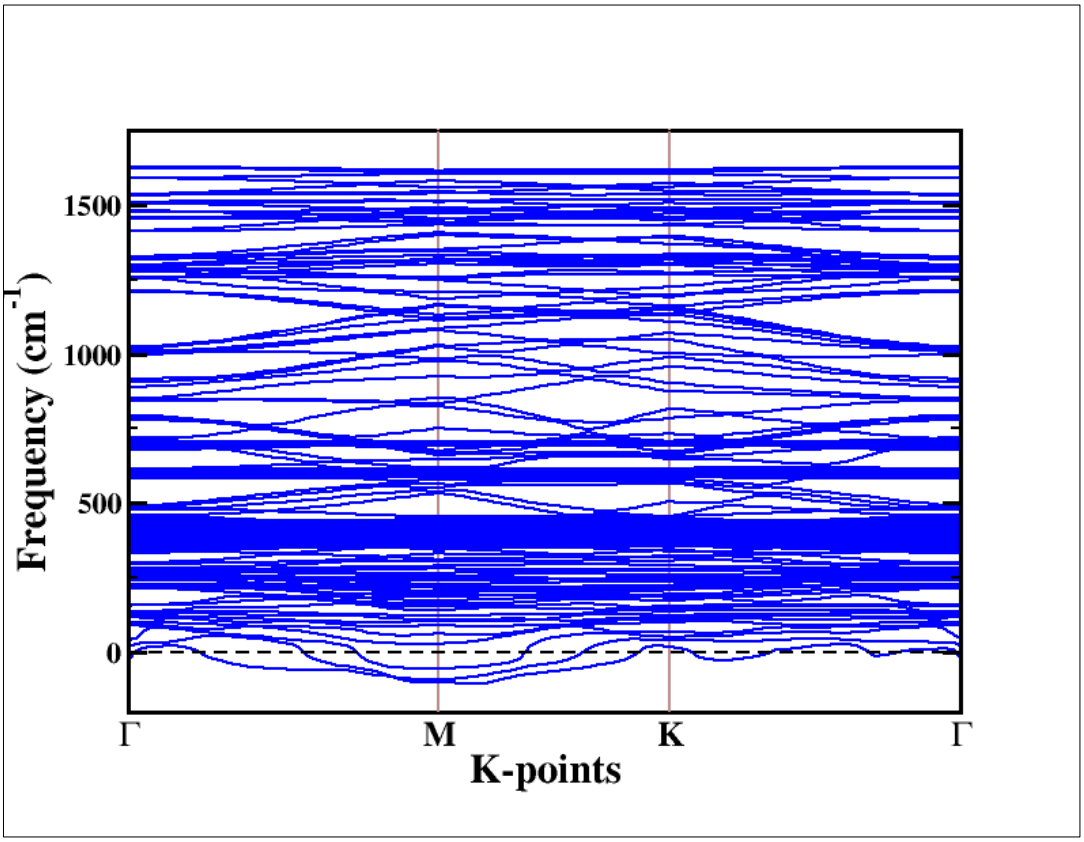


*Fig. S1 Calculated dispersion spectrums of $C_3N$/BP HS.*

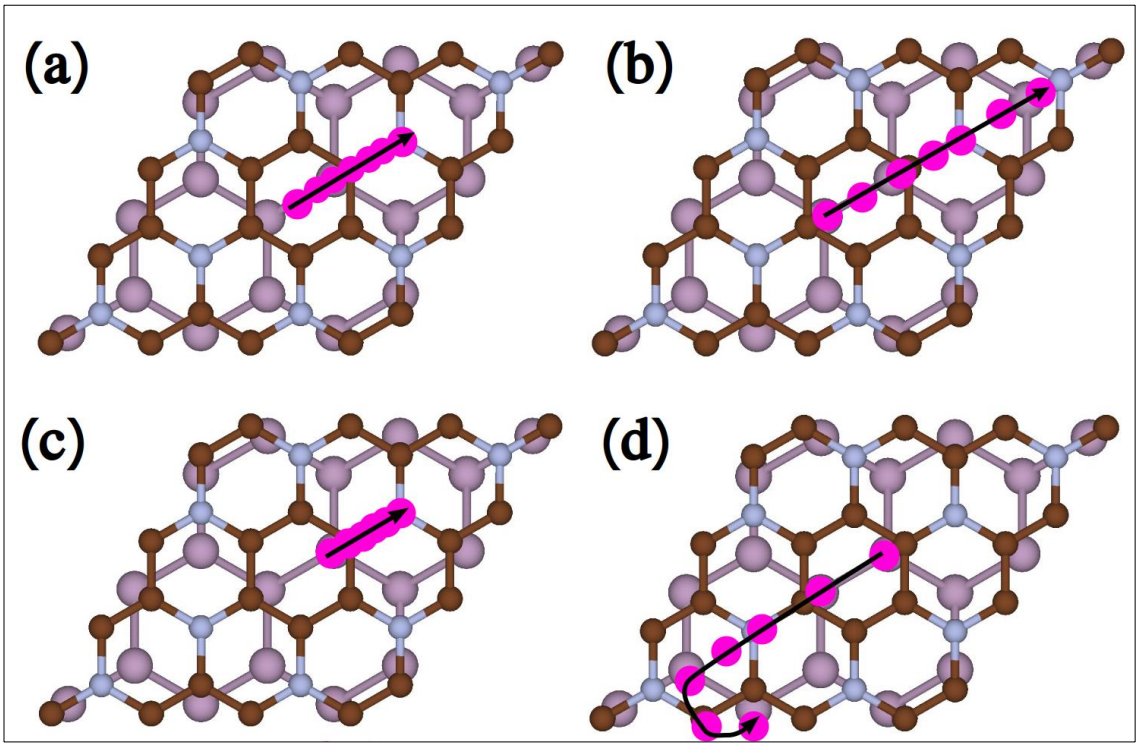


*Fig. S2 The migration pathways of X (Li/Na/K) in the interlayer of $C_3N$/BP HS.*

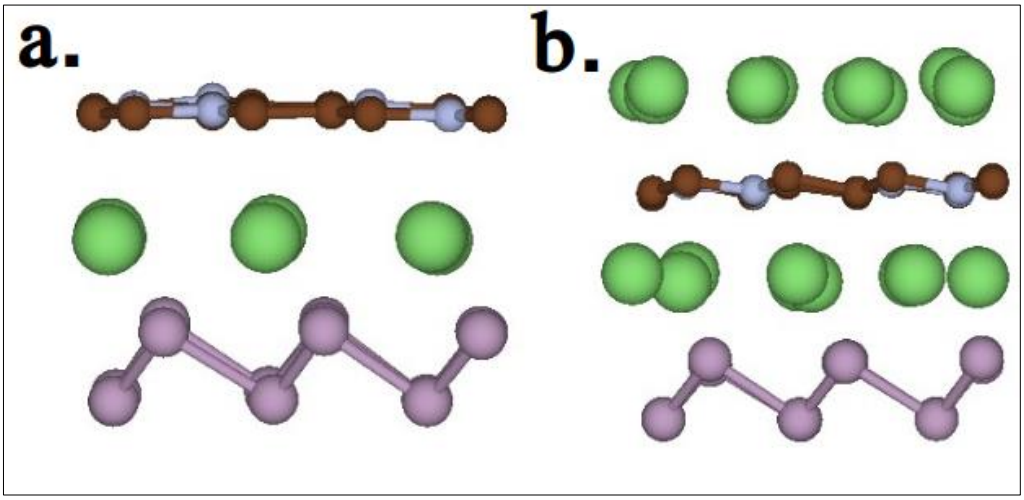


*Fig. S3 The optimized structures of Li inserted $C_3N$/BP HS. (a) $C_3N$/9Li/BP and (b) 16Li/$C_3N$/9Li/BP.*

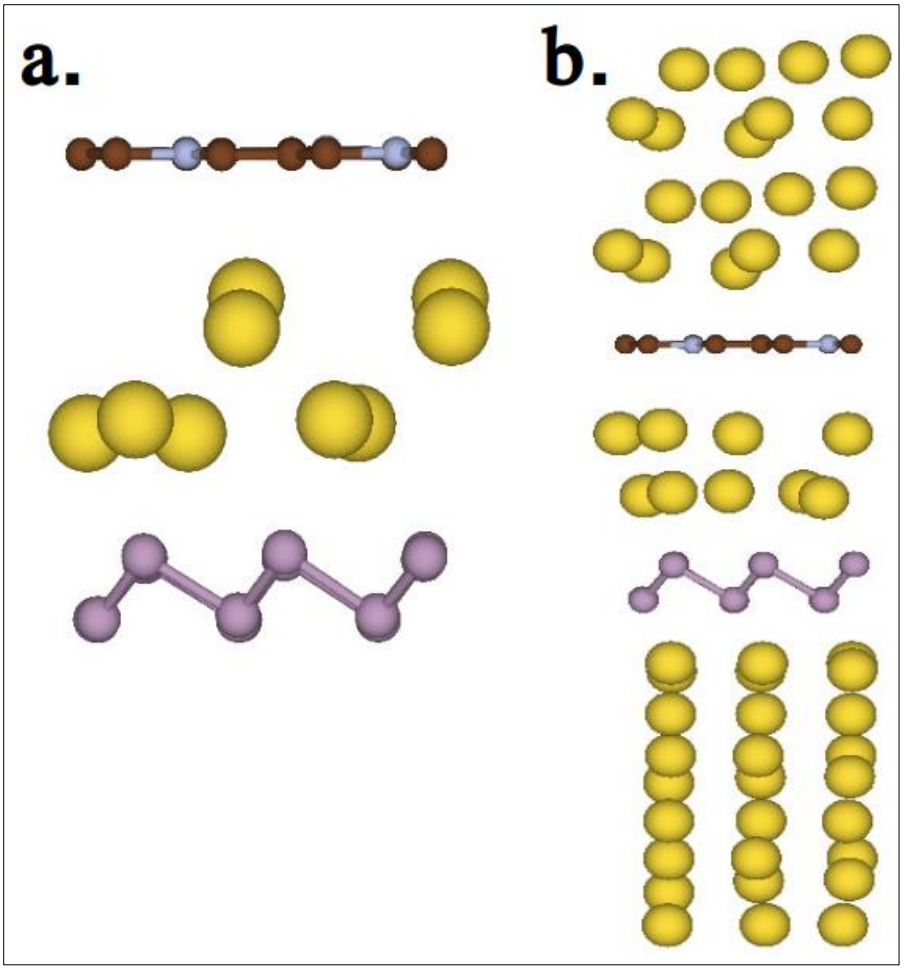


*Fig. S4 The optimized structures of Na inserted $C_3N$/BP HS. (a) $C_3N$/9Na/BP and (b) 18Na/$C_3N$/9Na/BP/27Na.*

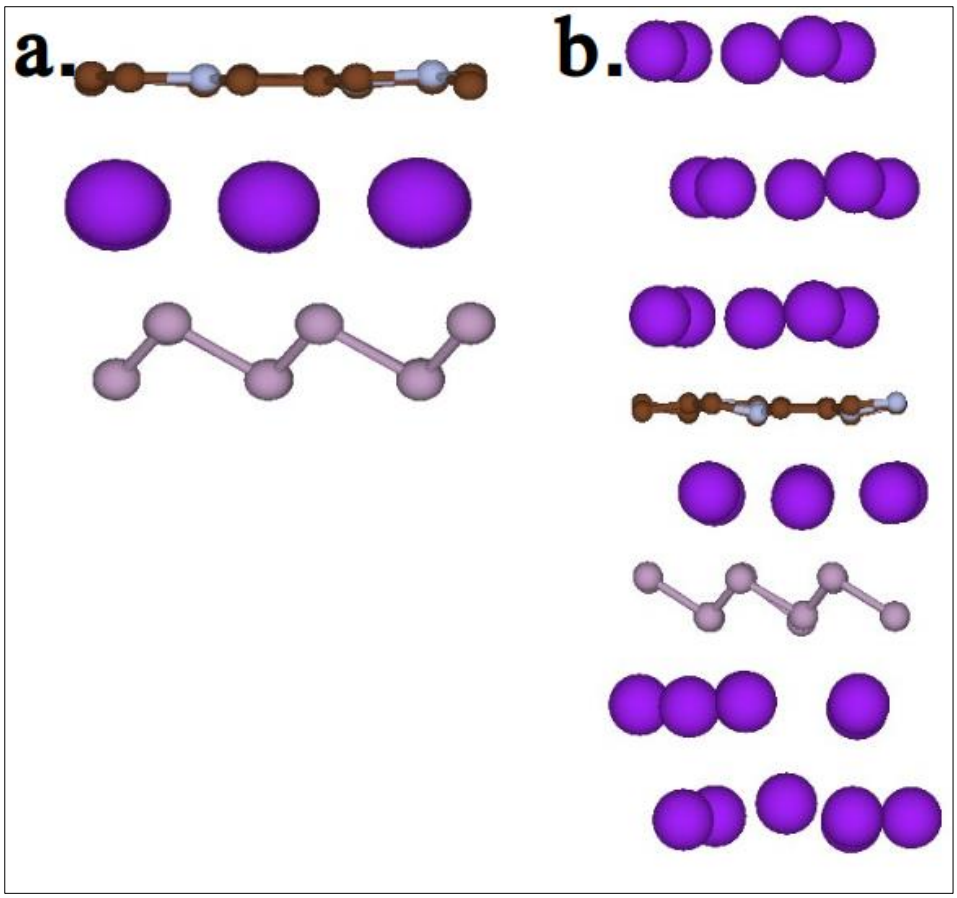


*Fig. S5 The optimized structures of K inserted $C_3N$/BP HS. (a) $C_3N$/9K/BP and (b) 15K/$C_3N$/9K/BP/12K.*