Supporting Information

Assembling Si$_2$BN nanoribbons to a 3D porous structure as a universal anode material for both Li- and Na-ion batteries with high performance

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Figure. S1 Energy hull of Si$_2$BN

Figure. S2 (a) Unit cell and 3×3×3 supercell of $\alpha$-3D-Si$_2$BN. (b) Unit cell and 3×3×3 supercell of $\beta$-3D-Si$_2$BN.
Figure. S3 (a-e) The partial density of states (PDOS) for Li-adsorption at site S$_1$-S$_5$ respectively.

Figure. S4 (a-e) The partial density of states (PDOS) for Na-adsorption at site S$_1$-S$_5$ respectively.
Figure. S5 Pictorial representation of charge density difference for (a) Lithium and (b) Sodium, at the second most stable site ($S_2$) in 3D-Si$_2$BN.

Figure. S6 The side views of six different concentrations of lithium ions in 3D-Si$_2$BN (a) 0.062 (b) 0.125 (c) 0.185 (d) 0.250 (e) 0.312 (f) 0.375
Figure. S7 The side view of four different concentrations of sodium ions in 3D-Si$_2$BN (a) 0.062 (b) 0.125 (c) 0.185 (d) 0.250

Figure. S8 (a) The AIMD simulation at room temperature for the following six different concentrations of lithium ions. (a) 0.062 (b) 0.125 (c) 0.185 (d) 0.250 (e) 0.312 (f) 0.375
Figure. S9 (a) The AIMD simulation at room temperature for the following four different concentrations of sodium ions. (a) 0.062 (b) 0.125 (c) 0.185 (d) 0.250

Figure. S10 Energy hull of NaSi$_2$BN during discharging
Figure S11 The AIMD exposed surface of the following six concentrations of lithium ions in 3D-Si$_2$BN (a) 0.062 (b) 0.125 (c) 0.185 (d) 0.25 (e) 0.312 (f) 0.375 at 300 K.
Figure. S12 The AIMD exposed surface of the following four concentrations of sodium ions in 3D-Si$_2$BN (a) 0.062 (b) 0.125 (c) 0.185 (d) 0.250 at 300 K.