Supporting Information

Assembling Si_2BN 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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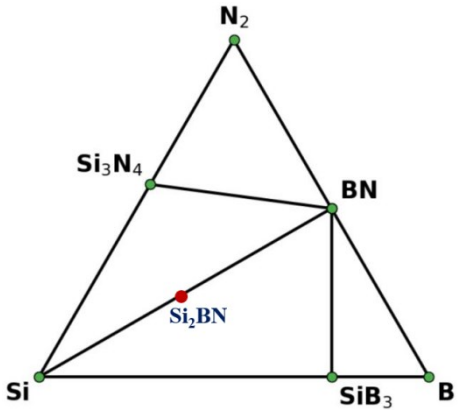

Figure. S1 Energy hull of Si_2BN

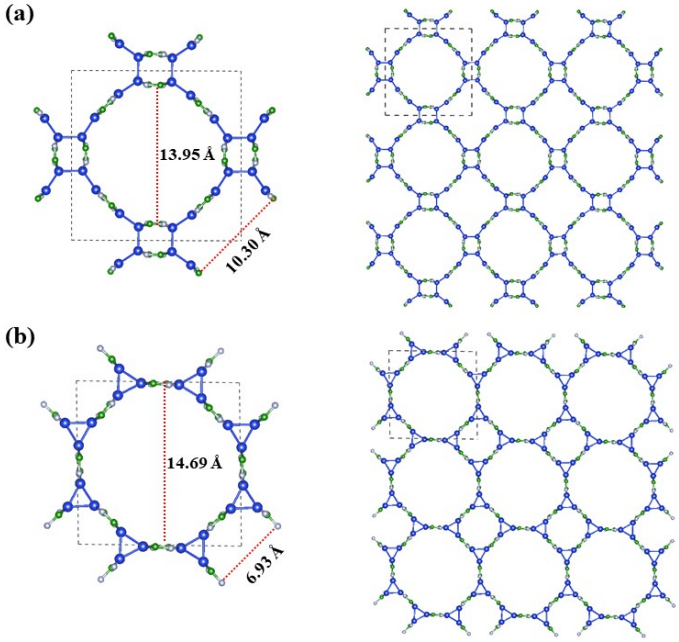

Figure. S2 (a) Unit cell and 3×3×3 supercell of α-3D-Si_2BN. (b) Unit cell and 3×3×3 supercell of β-3D-Si_2BN.

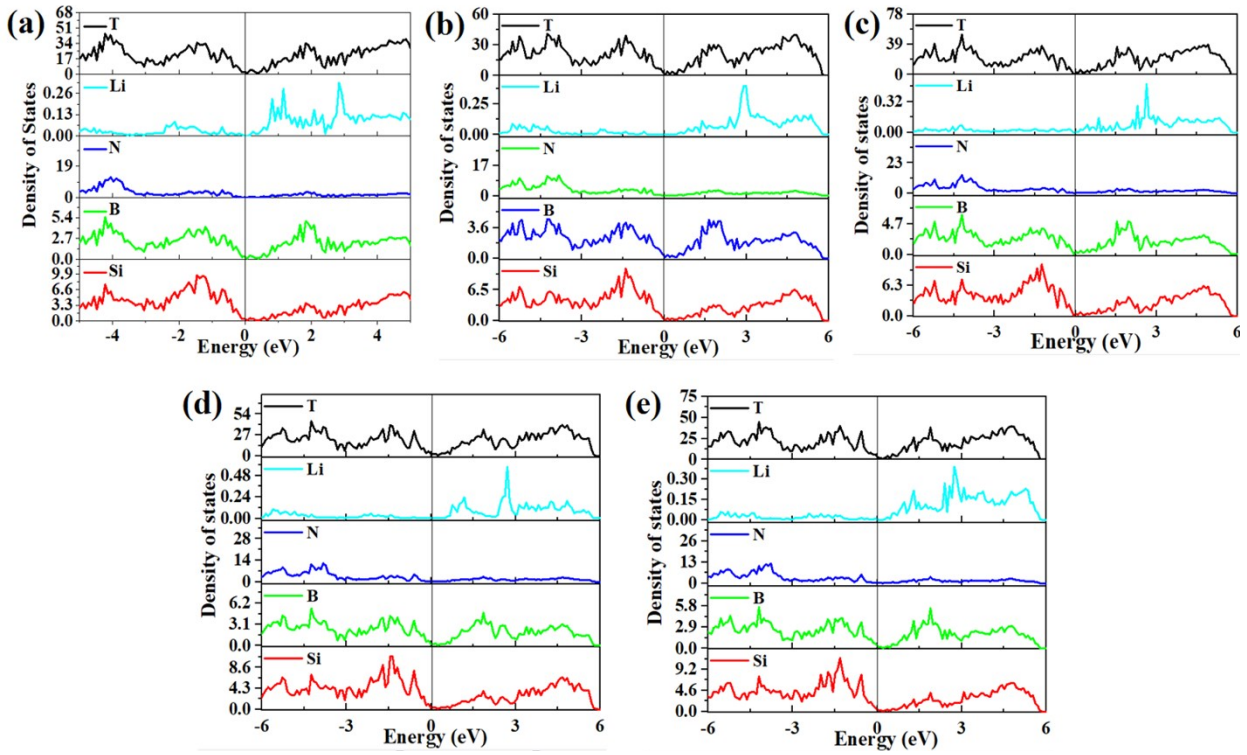

Figure. S3 (a-e) The partial density of states (PDOS) for Li-adsorption at site S_1-S_5 respectively.

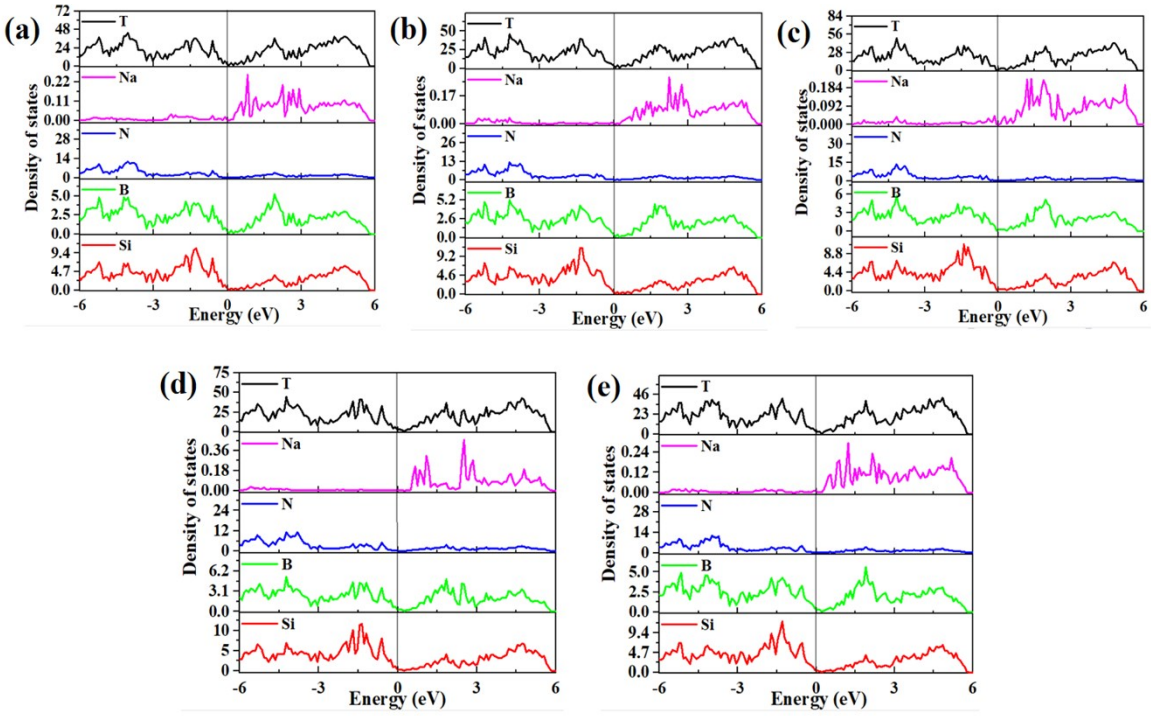

Figure. S4 (a-e) The partial density of states (PDOS) for Na-adsorption at site S_1-S_5 respectively.

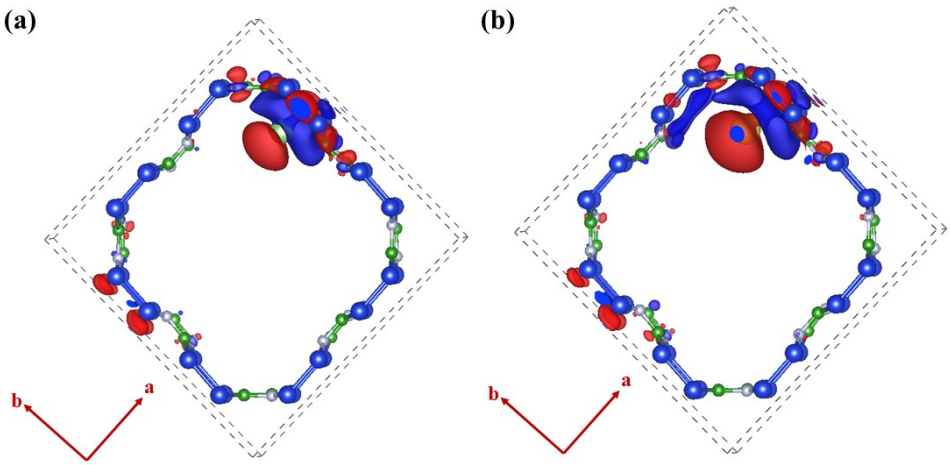

Figure. S5 Pictorial representation of charge density difference for (a) Lithium and (b) Sodium, at the second most stable site (S_2) in 3D-Si_2BN.

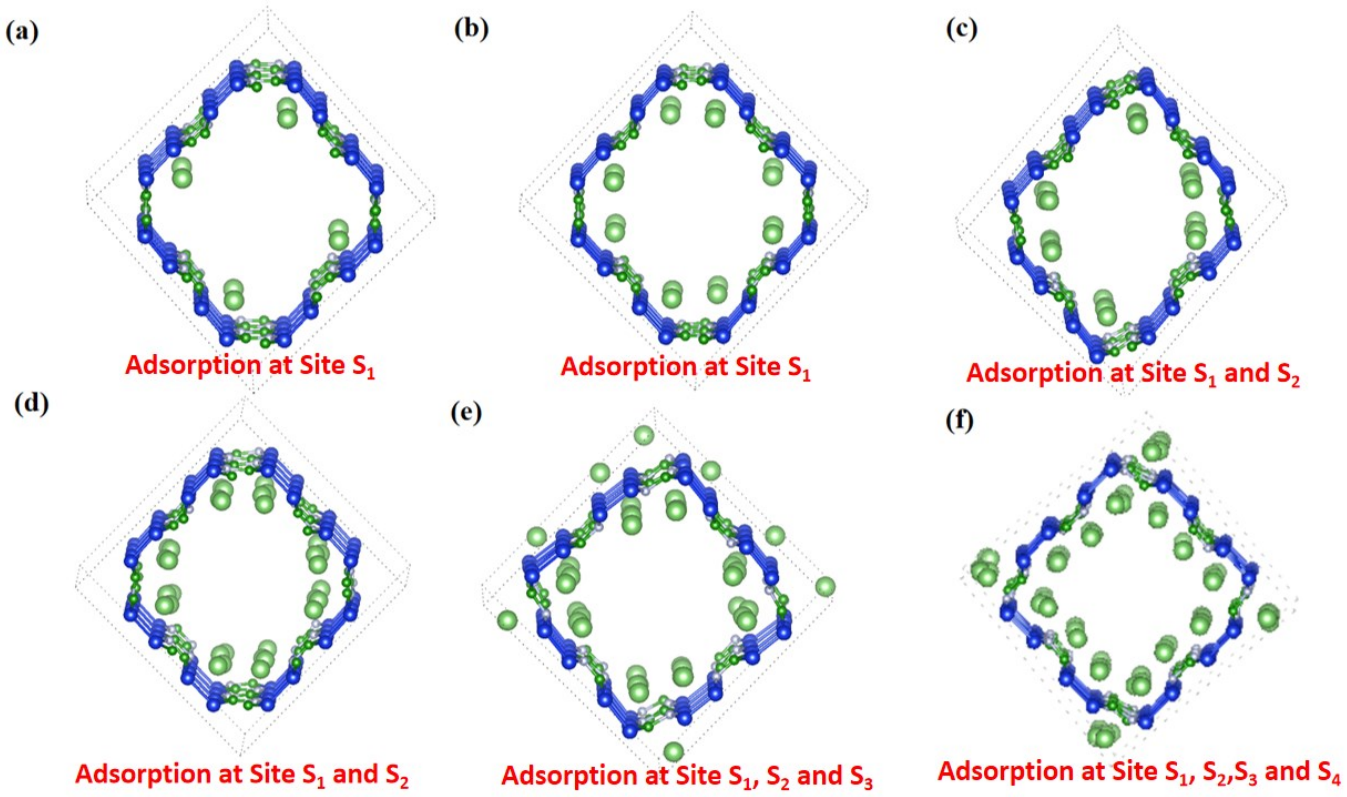

Figure. S6 The side views of six different concentrations of lithium ions in 3D-Si_2BN (a) 0.062 (b) 0.125 (c) 0.185 (d) 0.250 (e) 0.312 (f) 0.375

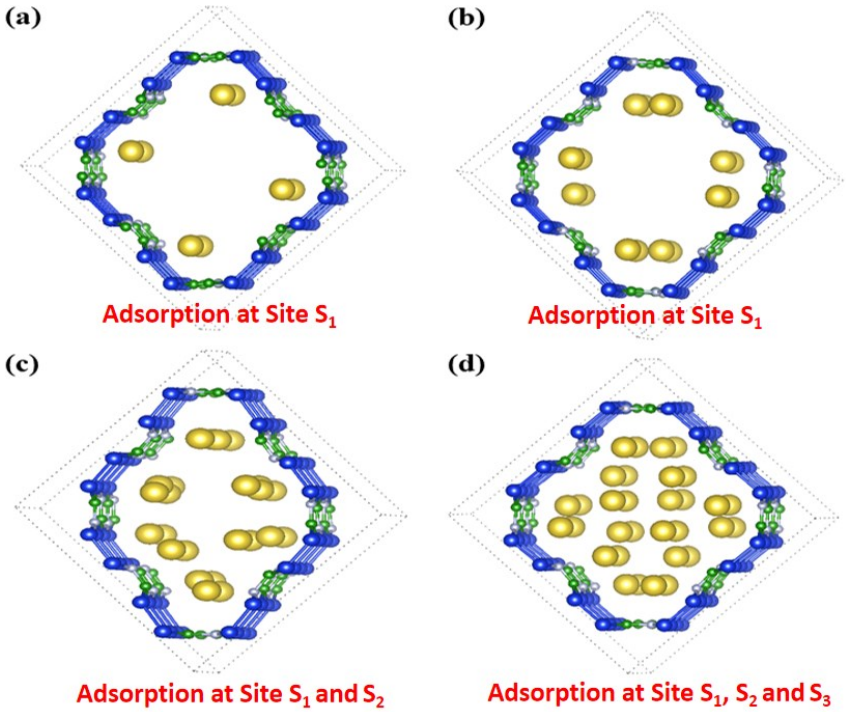

Figure. S7 The side view of four different concentrations of sodium ions in 3D-Si_2BN (a) 0.062 (b) 0.125 (c) 0.185 (d) 0.250

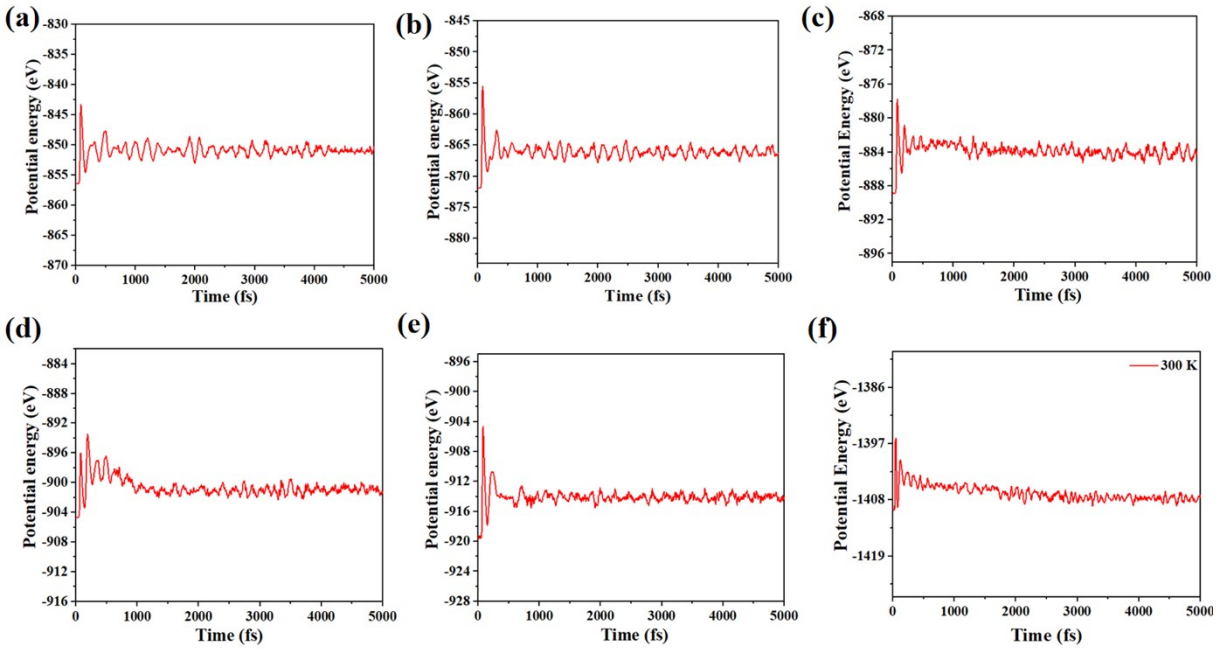

Figure. S8 (a) The AIMD simulation at room temperature for the following six different concentrations of lithium ions. (a) 0.062 (b) 0.125 (c) 0.185 (d) 0.250 (e) 0.312 (f) 0.375

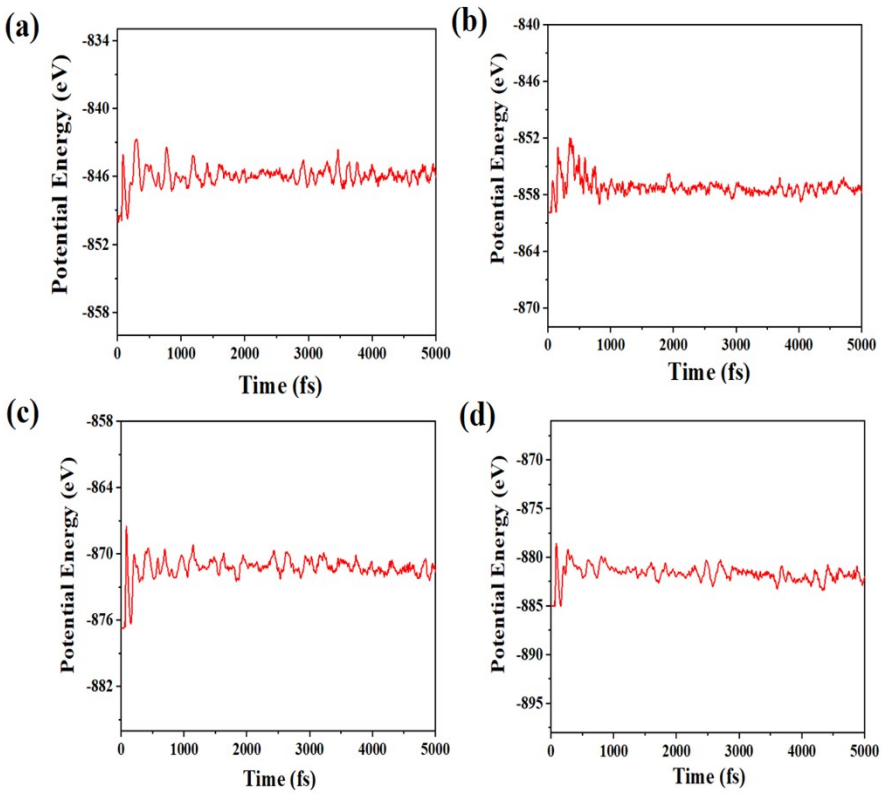

Figure. S9 (a) The AIMD simulation at room temperature for the following four different concentrations of sodium ions. (a) 0.062 (b) 0.125 (c) 0.185 (d) 0.250

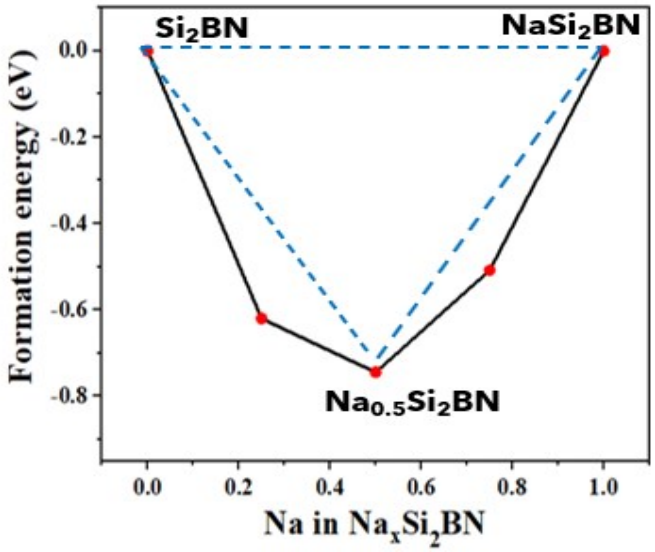

Figure. S10 Energy hull of $NaSi_2BN$ during discharging

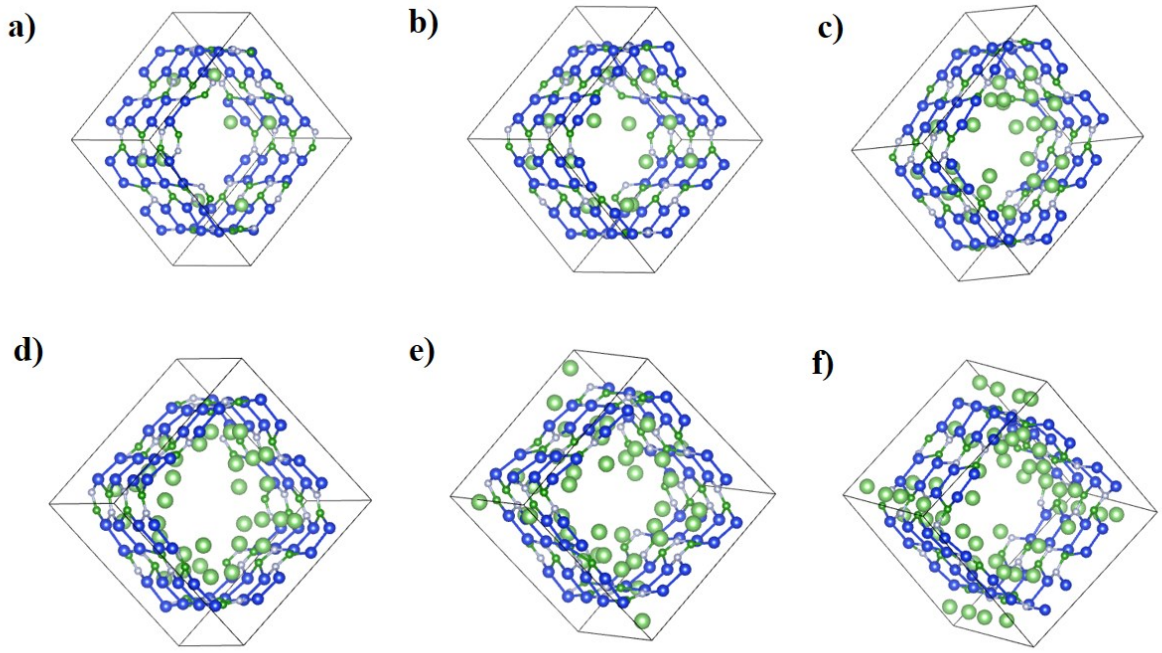

Figure. S11 The AIMD exposed surface of the following six concentrations of lithium ions in 3D-Si_2BN (a) 0.062 (b) 0.125 (c) 0.185 (d) 0.250 (e) 0.312 (f) 0.375 at 300 K.

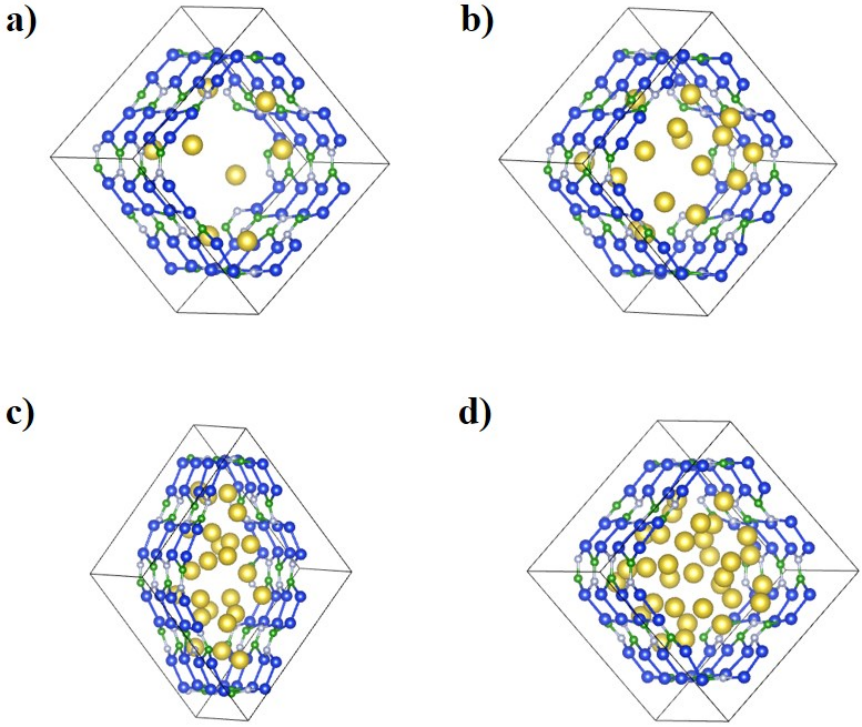

Figure. S12 The AIMD exposed surface of the following four concentrations of sodium ions in 3D-Si_2BN (a) 0.062 (b) 0.125 (c) 0.185 (d) 0.250 at 300 K.