Electronic Supplementary Material (ESI) for Dalton Transactions.

Support Information For

SiC_3N_3 Monolayer as a Universal Anode for Alkali Metal-ion Batteries

Xiaoying Xia,[a] Jianze Wu,[a] Xu Cai,[a] Bao Liu,[a] Zhaoxin Wang,[a] Yongfan Zhang,[a] Shuping Huang*[a,b]

[a] College of Chemistry, Fuzhou University, Fuzhou, 350108 Fujian, China

[b] Fujian Provincial Key Laboratory of Electrochemical Energy Storage Materials, Fuzhou, 350108 Fujian, China

*E-mail: huangshp@ gmail.com

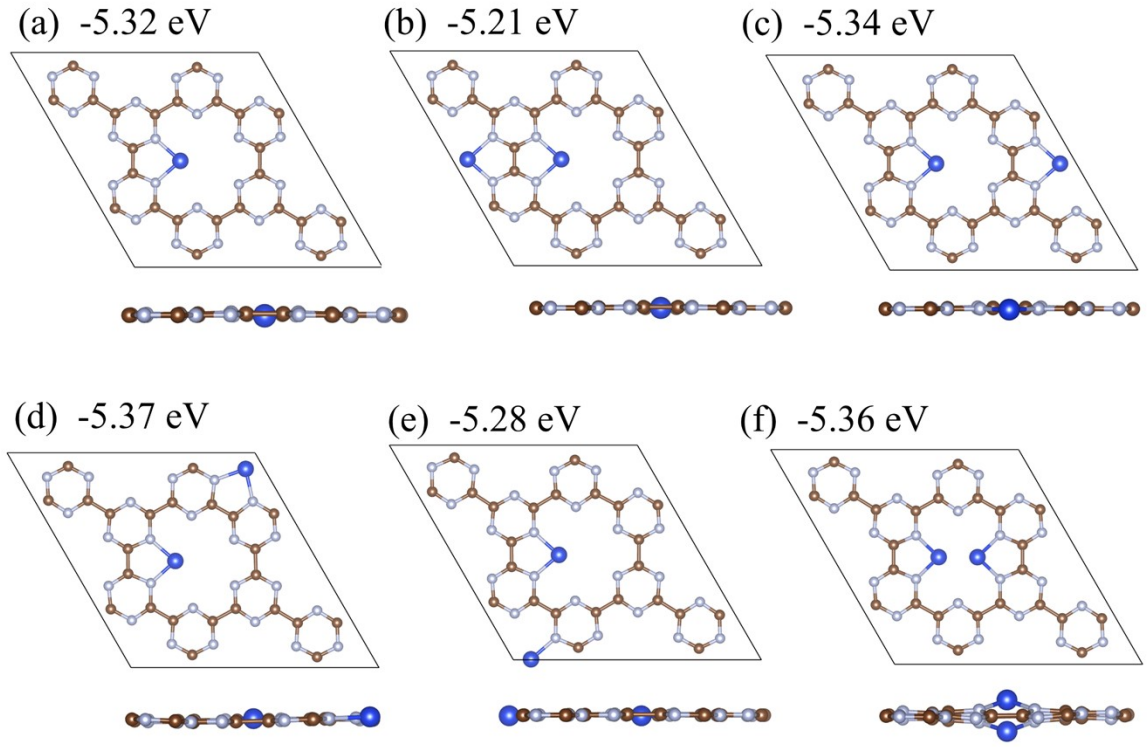

Fig. S1 The highly symmetric configurations of (a) $SiC_{24}N_{24}$ and (c-f) $SiC_{12}N_{12}$ and their corresponding formation energies.

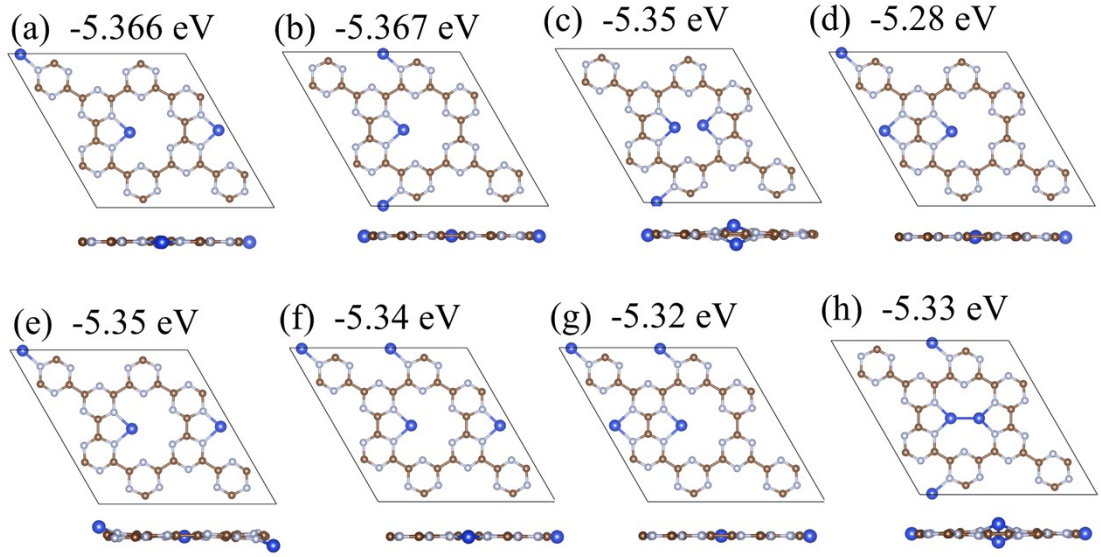

Fig. S2 The highly symmetric configurations of (a-e) SiC_8N_8 and (f-h) SiC_6N_6 and their corresponding formation energies.

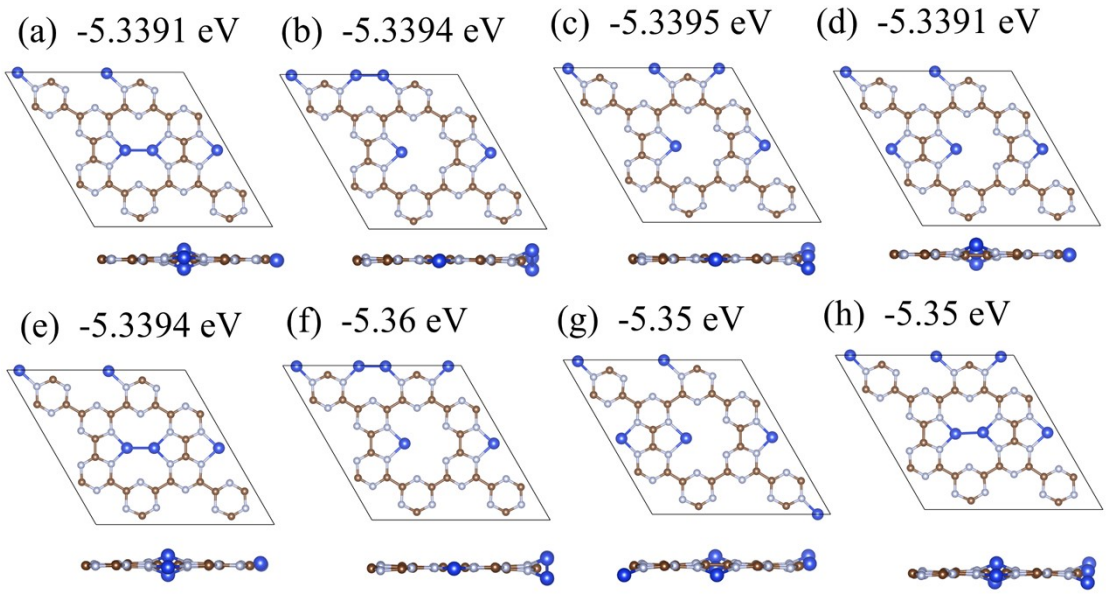

Fig. S3 The highly symmetric configurations of (a-e) $Si_5C_{24}N_{24}$ and (f-h) SiC_4N_4 and their corresponding formation energies.

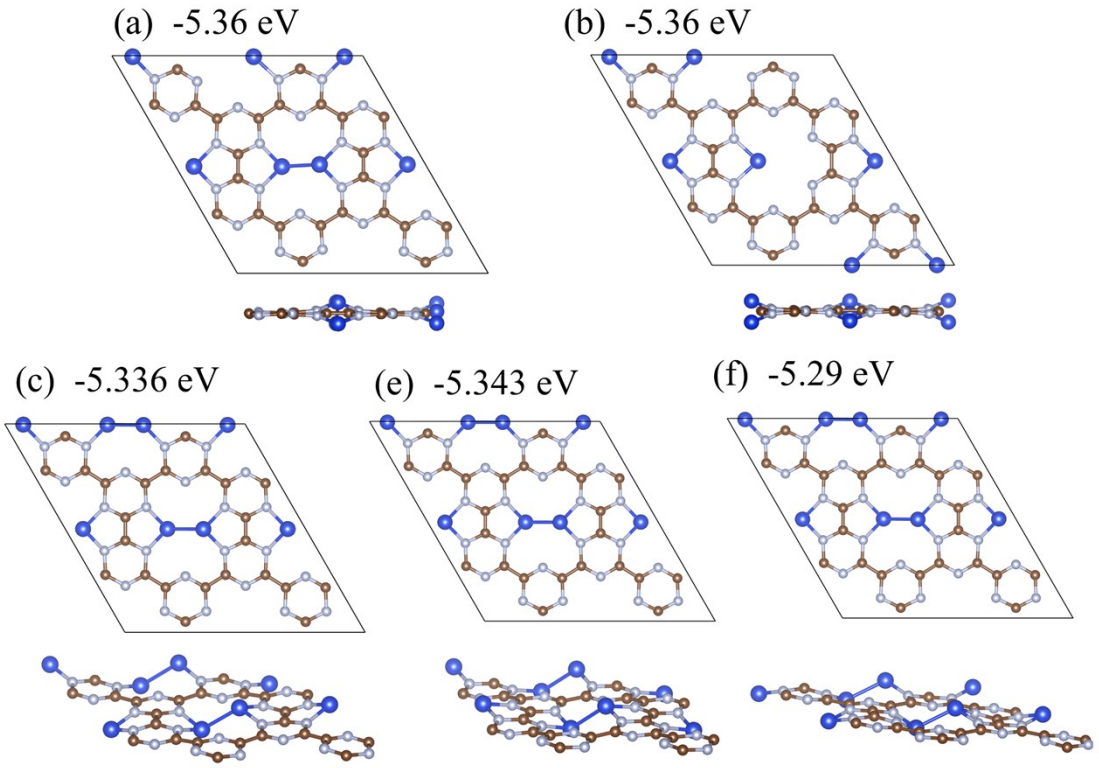

Fig. S4 The highly symmetric configurations of (a-b) $Si_7C_{24}N_{24}$ and (c-f) SiC_3N_3 and their corresponding formation energies.

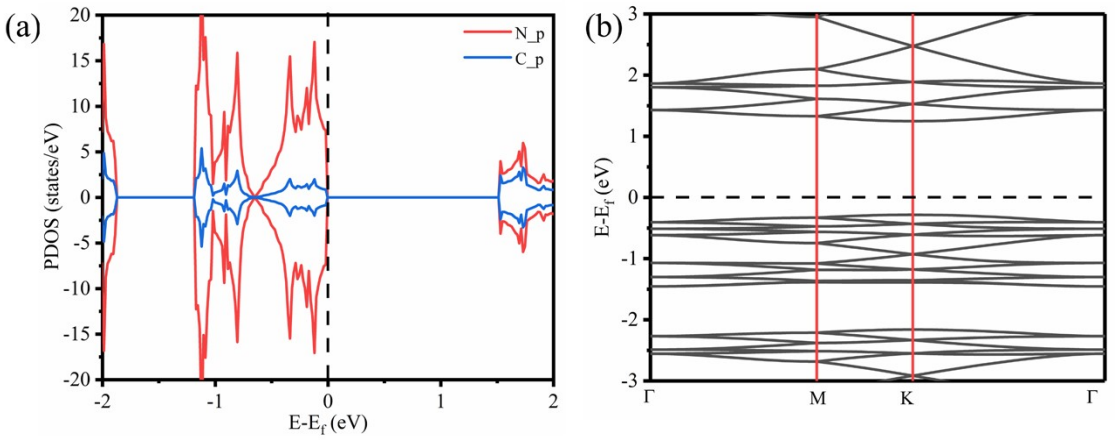

Fig. S5 (a) Partial density of states and (b) energy bands of g-CN.

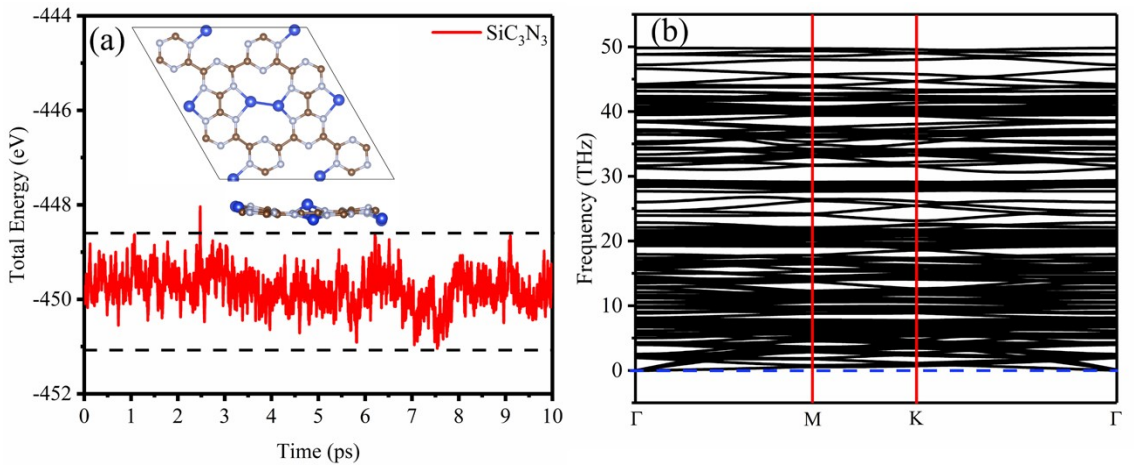

Fig. S6 (a) The fluctuation of total-energies, top and side-snapshots of SiC_3N_3 monolayer after AIMD simulation for 10 ps at 300 K. (b) Computed phonon dispersions of SiC_3N_3.

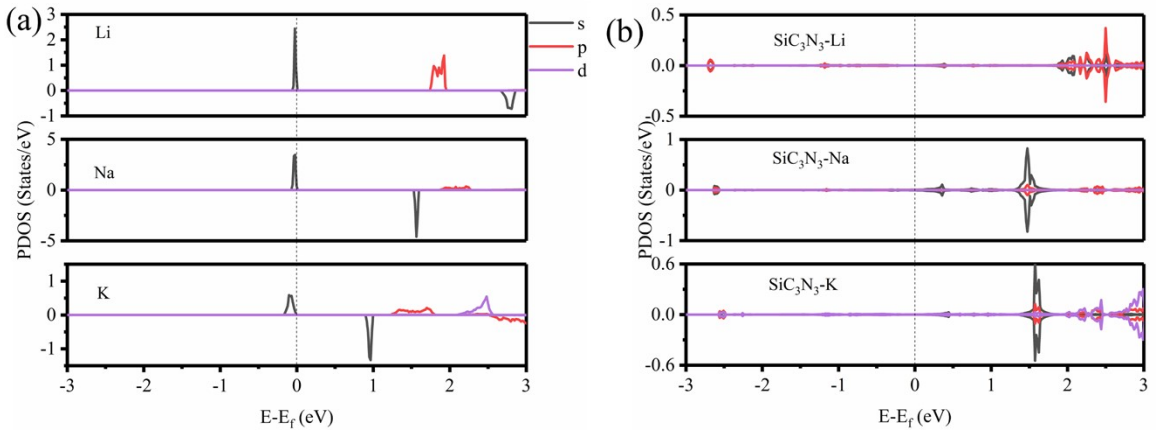

Fig. S7 The partial density of states of isolated Li, Na, and K. (b) The partial density of states of one Li, Na, and K adsorbed on SiC_3N_3.

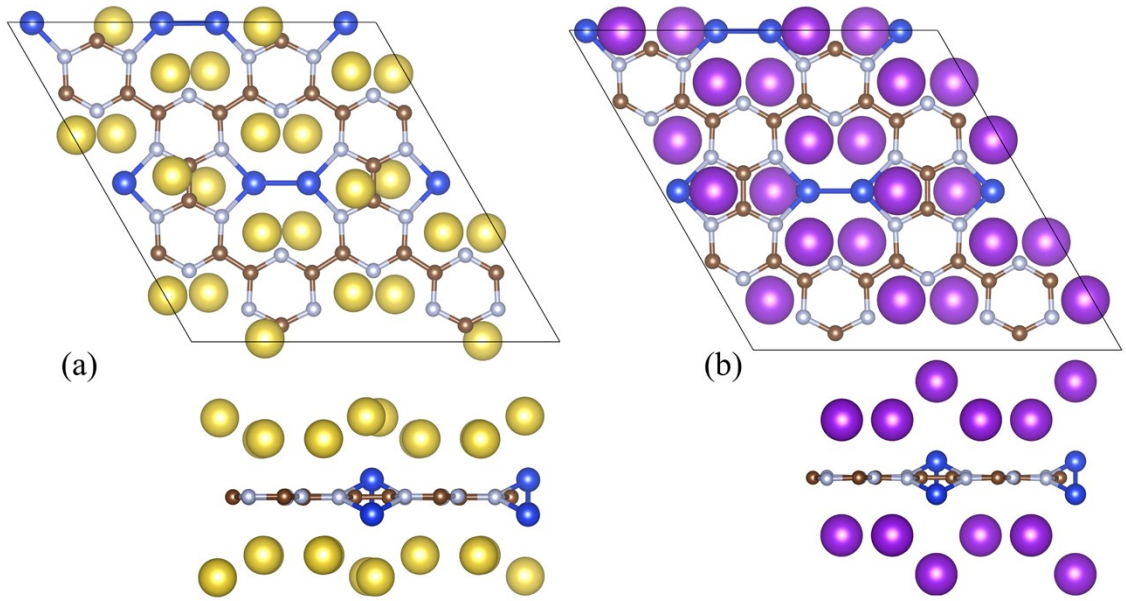

Fig. S8 The most stable configurations of (a) $Na_3SiC_3N_3$ and (b) $K_3C_3N_3$.

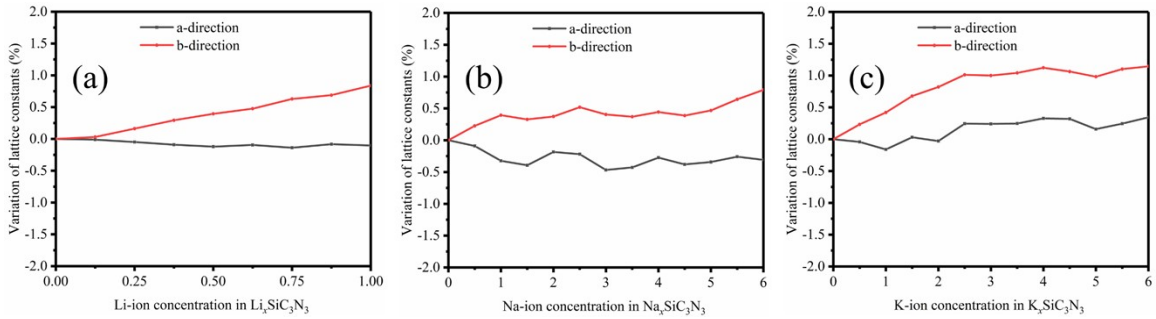

Fig. S9 Variation of lattice constants at different (a) Li, (b) Na and (c) K adsorption concentrations.