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

SUPPORTING INFORMATION

Computational determination of graphene-like TiB_4 monolayer for metal-ion batteries and nitrogen reduction electrocatalyst

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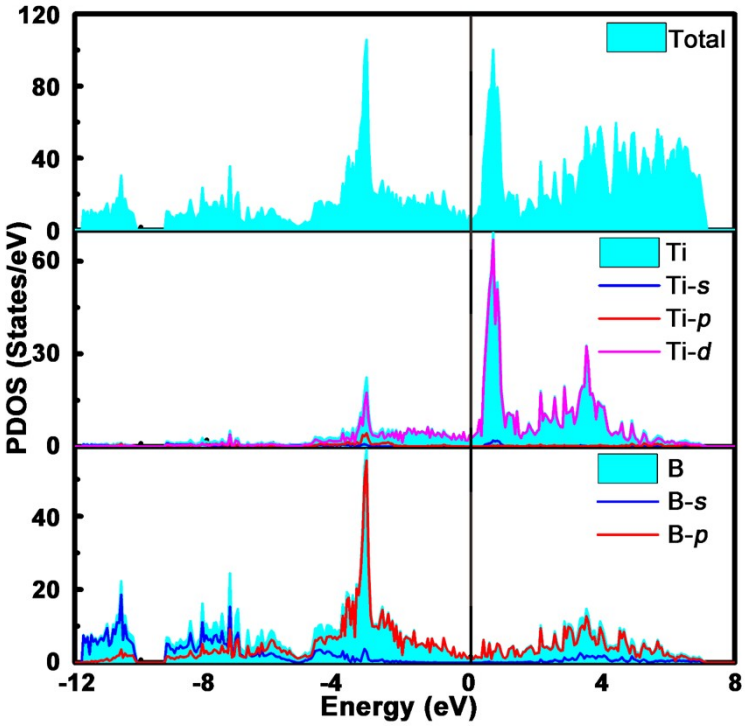

Fig. S1. The projected density of states (PDOS) of TiB_4 monolayer.

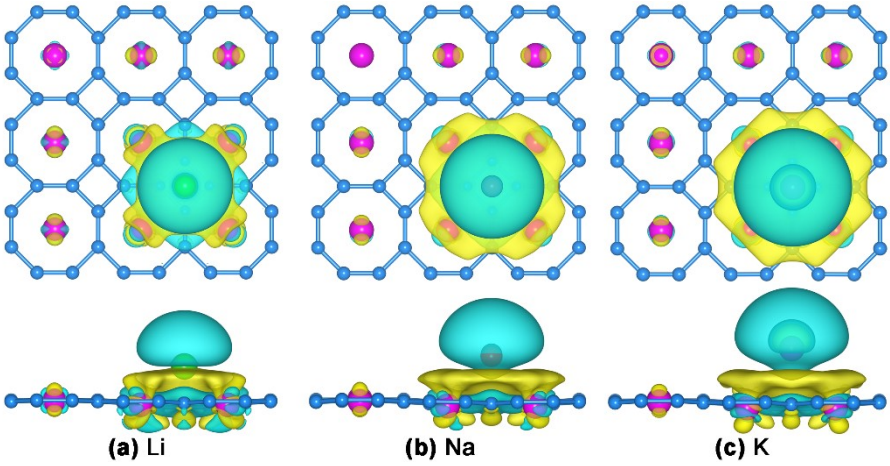

Fig. S2. The top and side views of charge density difference for single Li/Na/K ion on surfaces of TiB_4 monolayer. The iso-surface level is set to be 0.003 e/Å^3. The yellow and green regions denote the charge accumulation and depletion, respectively.

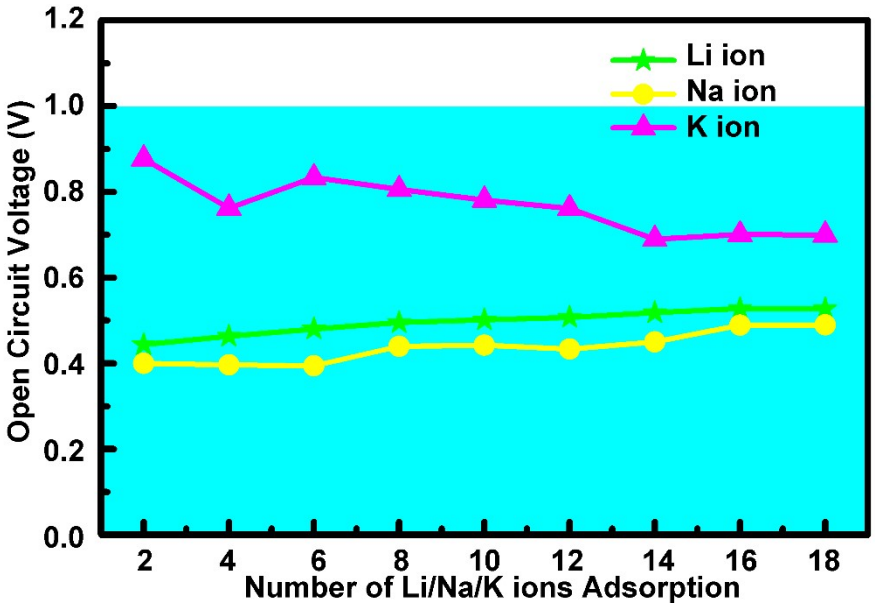

Fig. S3. The open circuit voltages as a function of the number of Li/Na/K ions adsorption on TiB_4 monolayer.

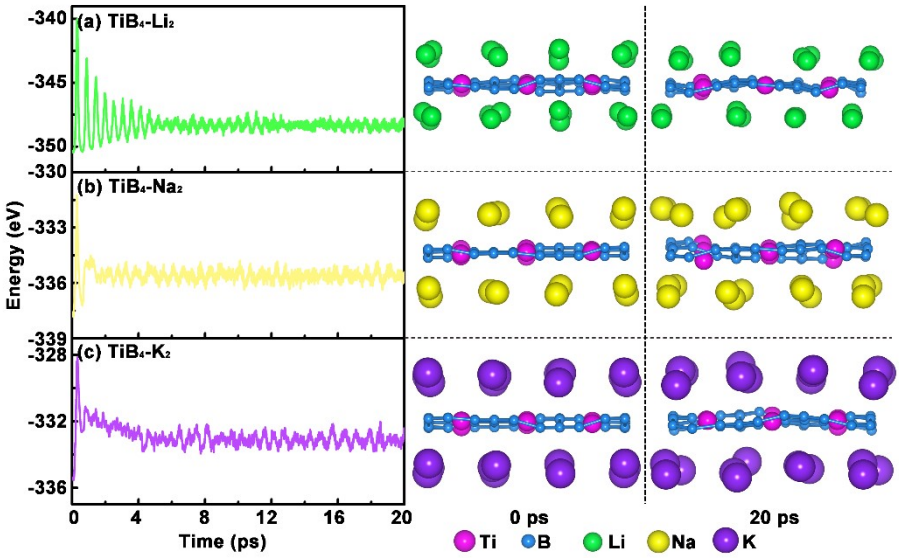

Fig. S4. The energy evolutions of (a) Li, (b) Na, (c) K ions absorbed on TiB_4 monolayer during AIMD simulations of 20 ps at 300 K. The corresponding structures at 0 and 20 ps are shown on the right panel.

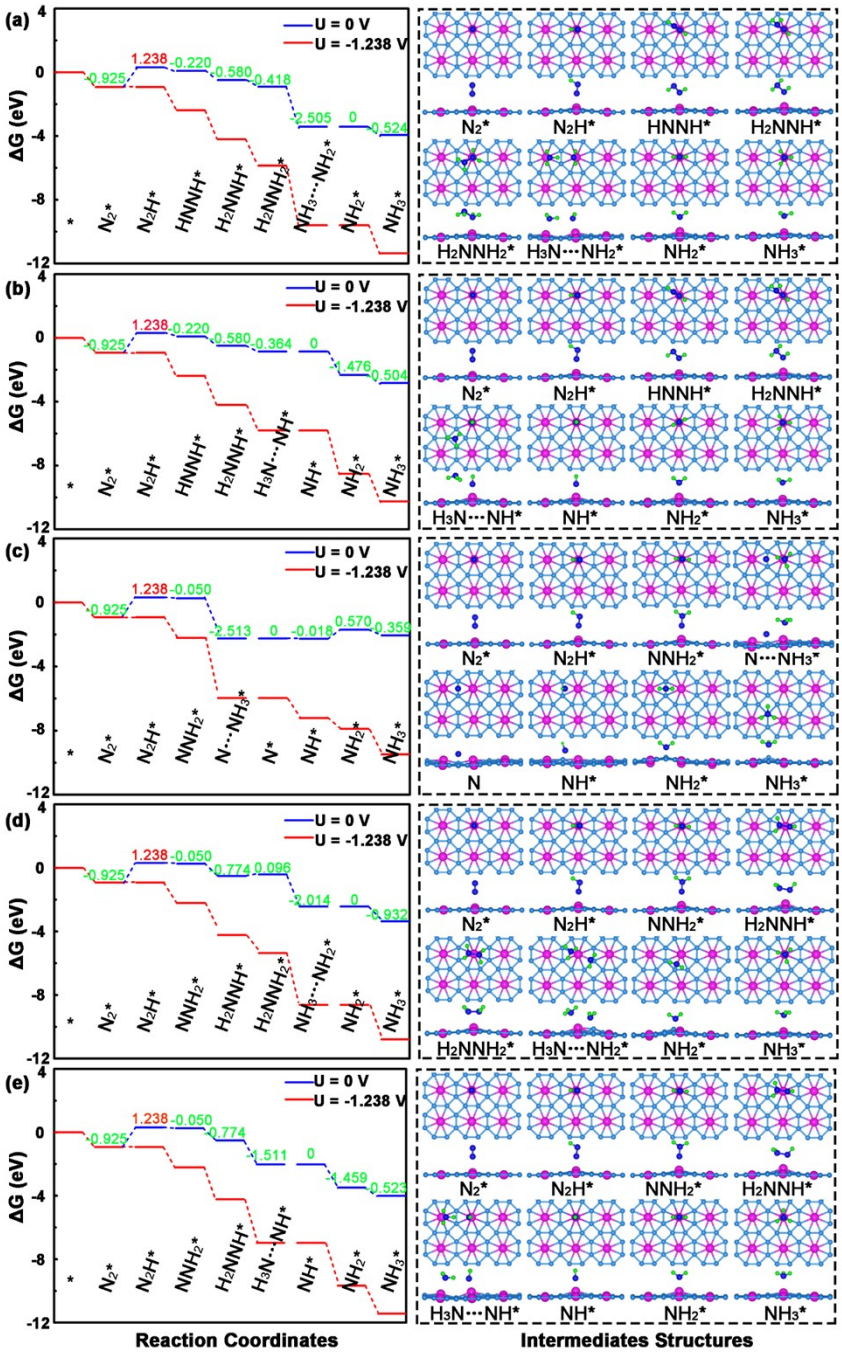

Fig. S5. The Gibbs free energy diagrams and corresponding structures of intermediates for N_2 conversion into NH_3 on TiB_4 monolayer *via* five different reaction pathways with end-on configurations, respectively. The symbol* denotes the intermediate adsorbed on the TiB_4 monolayer.

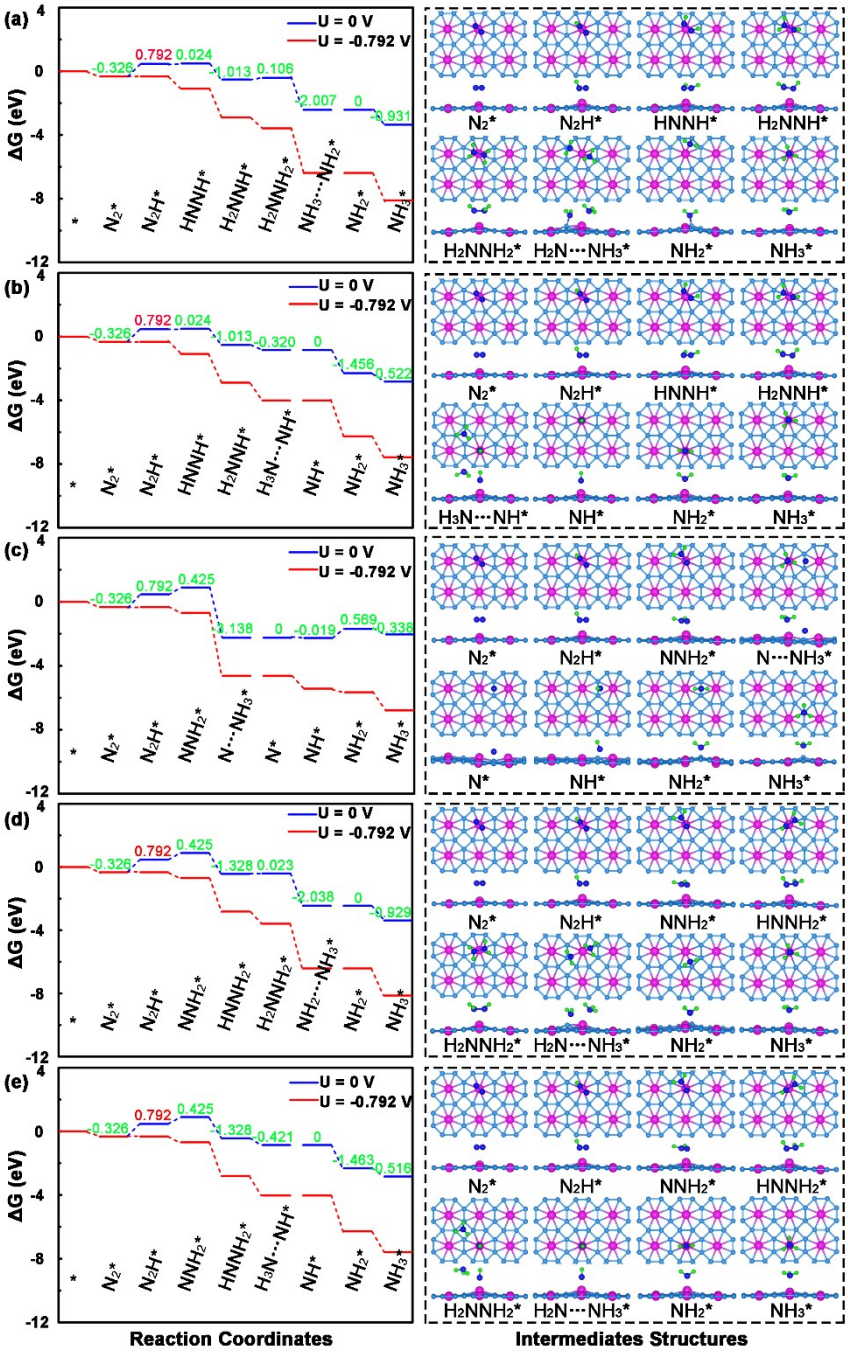

Fig. S6. The Gibbs free energy diagrams and corresponding structures of intermediates for N_2 conversion into NH_3 on TiB_4 monolayer *via* five different reaction pathways with side-on configurations, respectively. The symbol* denotes the intermediate adsorbed on the TiB_4 monolayer.

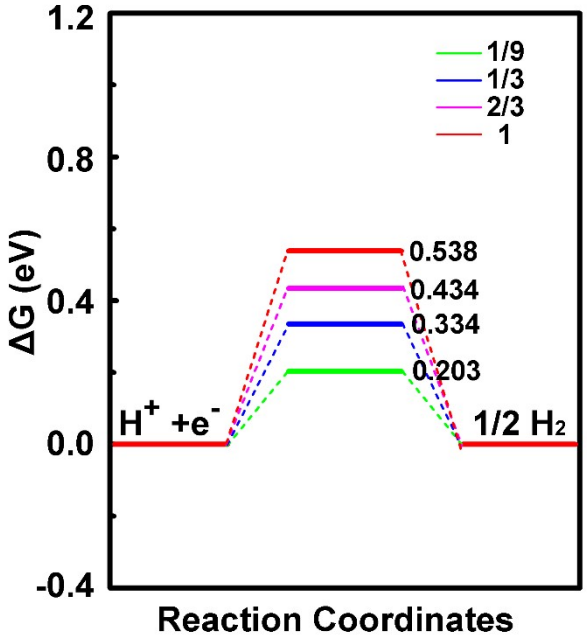

Fig. S7. The Gibbs free energy diagrams of different coverage hydrogen adsorption on TiB_4 monolayer. The green, blue, magenta, and red lines represent 1/9, 1/3, 2/3, and 1 coverage, respectively.