Electronic Supplementary Information

Ti_2PTe_2 Monolayer: A Promising Two-Dimensional Anode Material for Sodium-Ion Batteries

Jie Liu,[†] Man Qiao,[†] Xiaorong Zhu,[†] Yu Jing,[‡,§]* Yafei Li[†]*

[†]Jiangsu Key Laboratory of New Power Batteries, Jiangsu Collaborative Innovation Centre of Biomedical Functional Materials, School of Chemistry and Materials Science, Nanjing Normal University, Nanjing 210023, China

[‡]College of Chemical Engineering, Nanjing Forestry University, Nanjing 210037, China

[§]Jiangsu Co-Innovation Centre of Efficient Processing and Utilization of Forest Resources, Nanjing 210037, China

To whom correspondence should be addressed. Email: yujing@njfu.edu.cn (YJ) and liyafei@njnu.edu.cn (YL)

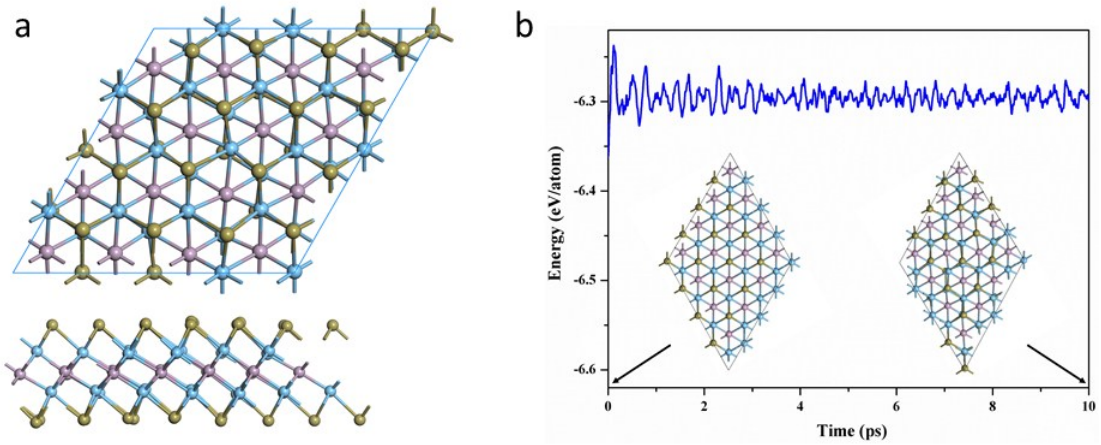

Fig. S1 (a) Snapshots of the equilibrium structures of Ti_2PTe_2 monolayer at the end of a 10 ps ab initio molecular dynamic (AIMD) simulation at the temperature of 500 K. (b) The evolution of the total energy of AIMD simulations.

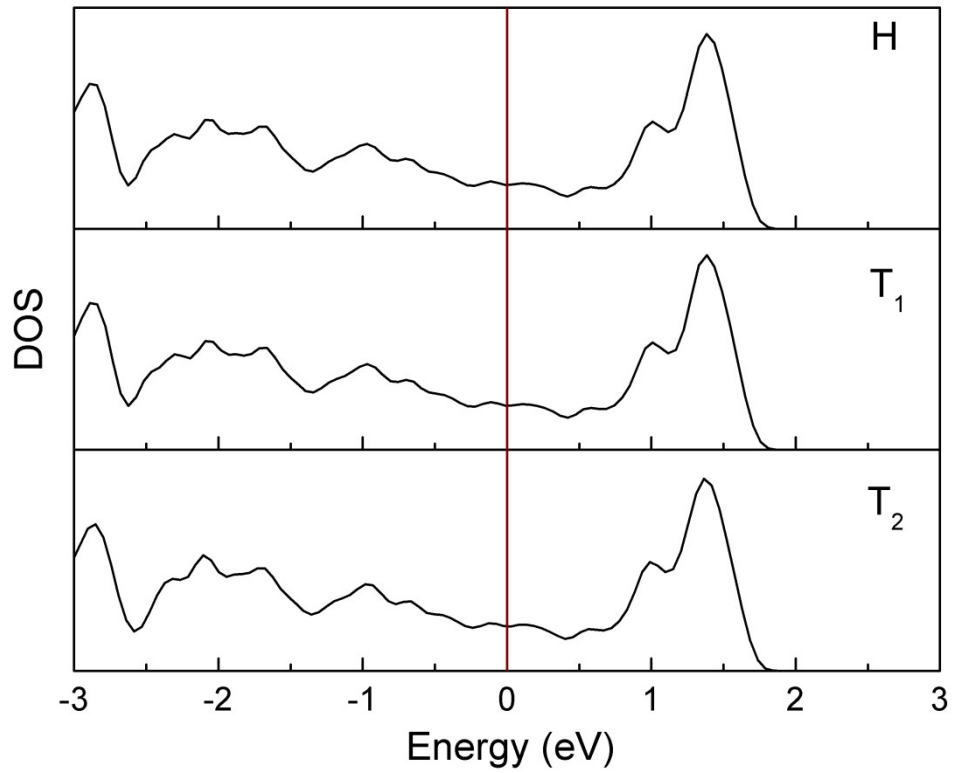

Fig. S2 Electric density of states (DOS) of Ti_2PTe_2 monolayer after Na adsorption.

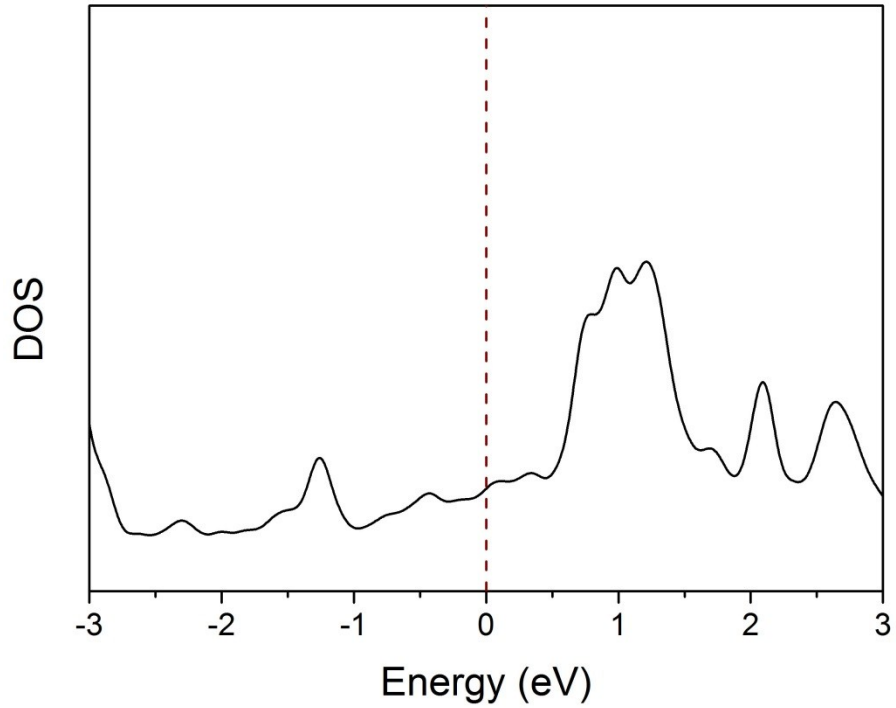

Fig. S3 Electric density of states (DOS) of Ti_2PTe_2 monolayer after adding two Na layers on both sides.