Electronic Supplementary Material (ESI) for Nanoscale.

The S-functionalized Ti_3C_2 Mxene as a High Capacity Electrode Material for Na-ion Batteries: A DFT Study

Qiangqiang Meng,[a,b] Jiale Ma,[a] Yonghui Zhang,[a] Zhen Li,[a] Chunyi Zhi,[a] Alice Hu,[c] and Jun Fan*[a,d]

[a] Department of Materials Science& Engineering, City University of Hong Kong, Hong Kong, China Email: junfan@cityu.edu.hk.

[b] Key Laboratory for Advanced Technology in Environmental Protection of Jiangsu Province, Yancheng Institute of Technology, Yancheng, Jiangsu 224051, China.

[c] Department of Mechanical and Biomedical Engineering, City University of Hong Kong, Hong Kong, China

[d] City University of Hong Kong Shenzhen Research Institute, Shenzhen 518057, China

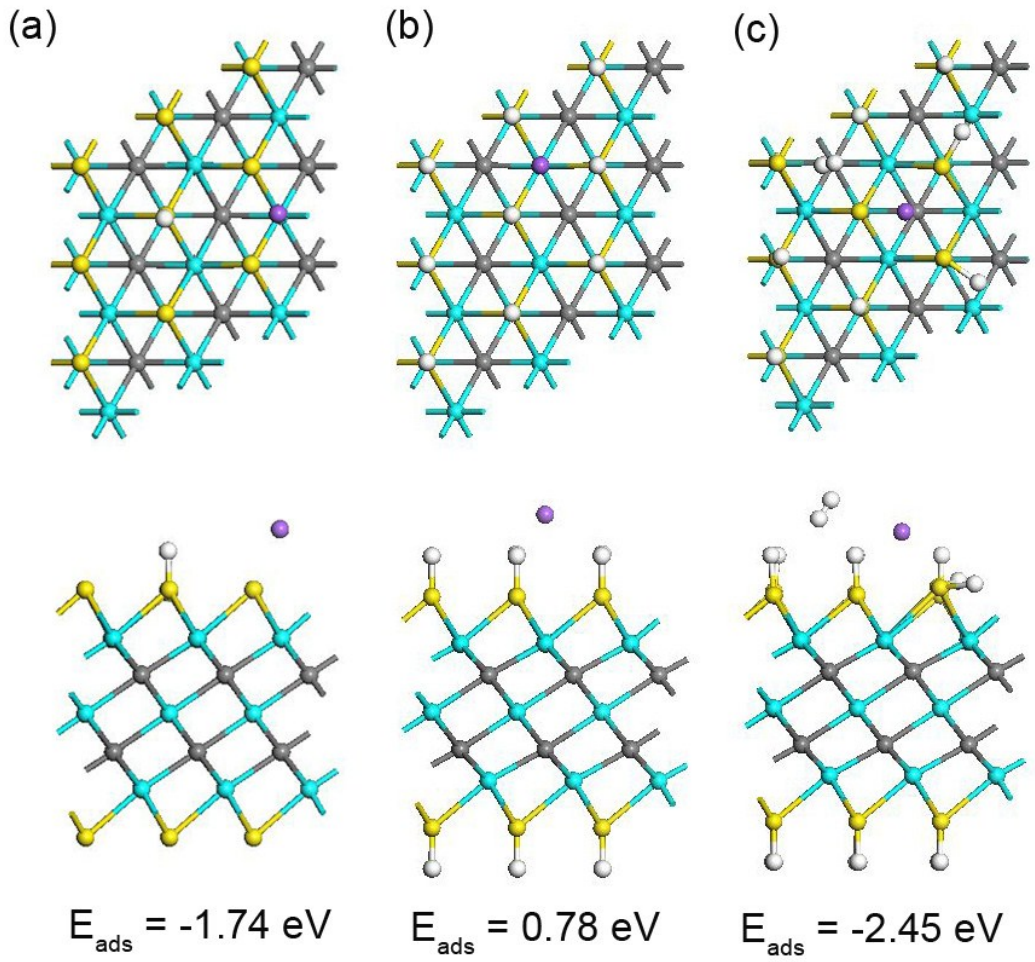

Figure S1. Geometric structures and related adsorption energies for Na adsorption on Hydrogenated $Ti_3C_2S_2$ monolayer of top and side views: (a) Low coverage Hydrogenated $Ti_3C_2S_2$ monolayer; (b-c) Full coverage Hydrogenated $Ti_3C_2S_2$ monolayer with different initial distance between Na atom, respectively.

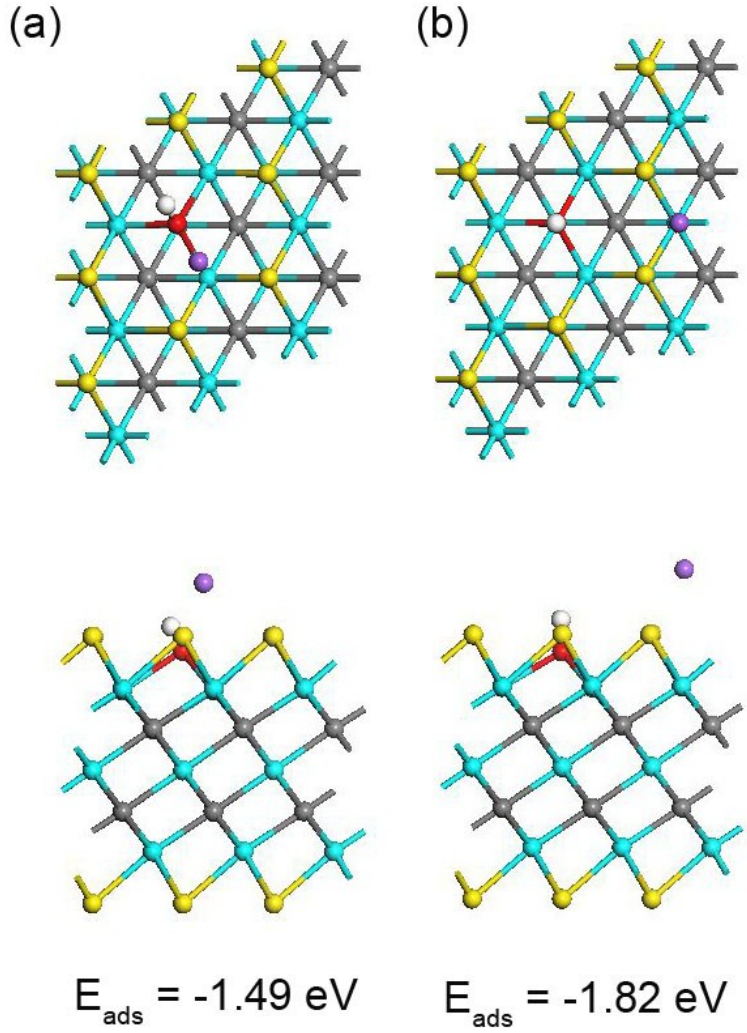

Figure S2. Geometric structures and related adsorption energies for Na adsorption on Hydroxylated $Ti_3C_2S_2$ monolayer of top and side views: (a) Nearby the OH group; (b) Far away from the OH group.

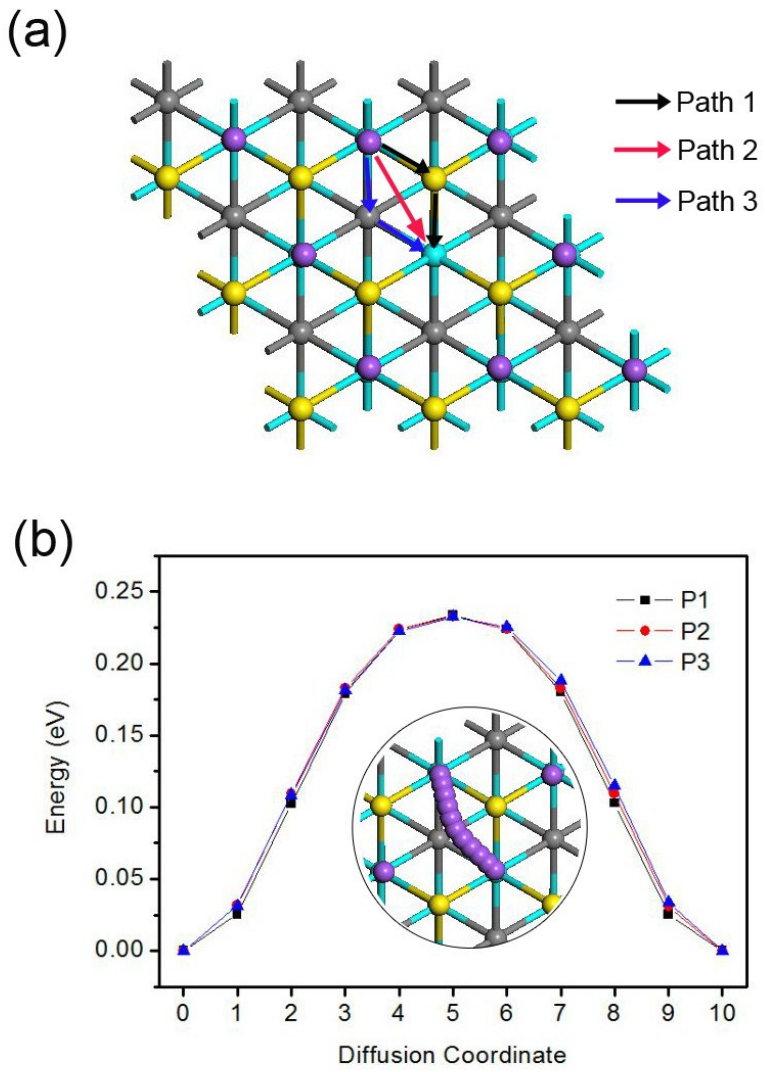

Figure S3. (a) Considered migration paths of Na diffusion on the $Ti_3C_2S_2$ monolayer with high Na coverage, meanwhile P1, P2, and P3 represent possible migration paths for Na atoms; (b) the migration paths and corresponding diffusion energy barrier profiles.

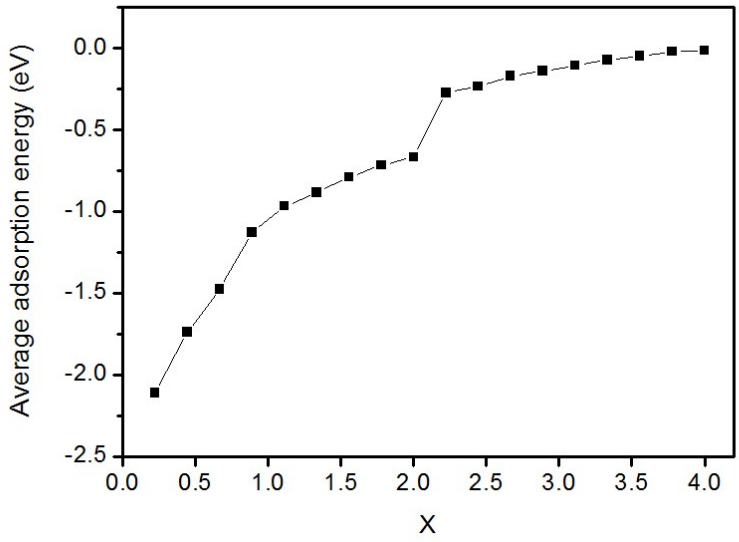

Figure S4. The average adsorption energy of Na atoms as a function of x in $Ti_3C_2S_2Na_x$.