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

This journal is © the Owner Societies 2023

Supplementary Material of:

Two-dimensional TiCl₂: A high-performance anode material for Na-ion batteries with high

capacity and fast diffusion

Hong-Yao Zhu, a Xiao-Juan Ye, a Lan Meng, a Xiao-Hong Zheng, Ban Jia, Chun-Sheng Liua,*

^aCollege of Electronic and Optical Engineering, Nanjing University of Posts and

Telecommunications, Nanjing 210023, China

^bCollege of Information Science and Technology, Nanjing Forestry University, Nanjing 210037,

China

^cInstitute of Theoretical Chemistry, College of Chemistry, Jilin University, Changchun 130023,

China

Email: csliu@njupt.edu.cn

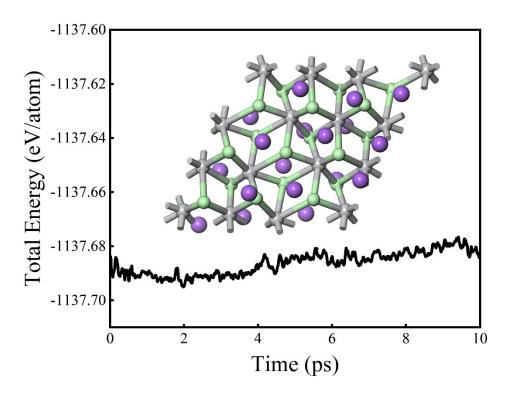


Fig. S1. Total energy evolution of Na₂TiCl₂ at 300 K. The inset is the snapshot of the final configuration from the top view.

 $\textbf{Table S1.} \ \ \text{Calculated differential adsorption energy } (E_{\text{diff-ads}}) \ \ \text{with different numbers of Na adsorbed on TiCl}_2.$

Number of Na atoms adsorbed on TiCl ₂	$E_{ m diff}$ - ads (eV)
1	-1.48
2	-1.36
3	-1.18
4	-1.26
5	-1.21
6	-1.24
7	-1.19
8	-1.16
9	-1.23
10	-1.15
11	-1.20
12	-1.18
13	-1.17
14	-1.15
15	-1.19
16	-1.18
17	-1.21
18	-1.16
19	0.14