Electronic Supplementary Material (ESI) for Energy and Environmental Science

Supporting information for

Atomic-scale investigation on lithium storage mechanism in $TiNb_2O_7$

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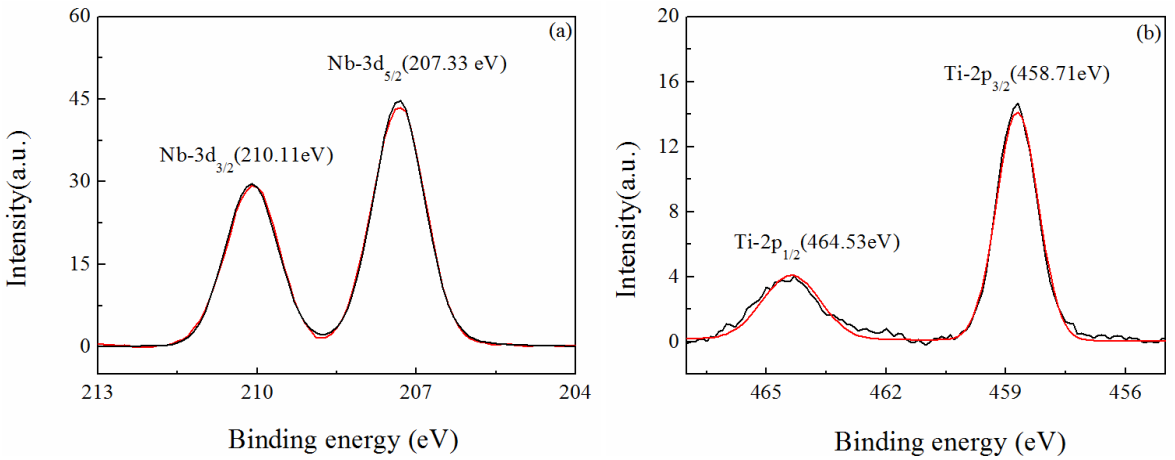

Figure S1 Narrow-scan XPS spectra of (a) Nb 3d, (b) Ti 2p in $TiNb_2O_7$. It shows that the chemical states of Nb and Ti are + 5 and + 4 in the pure $TiNb_2O_7$ sample, respectively.

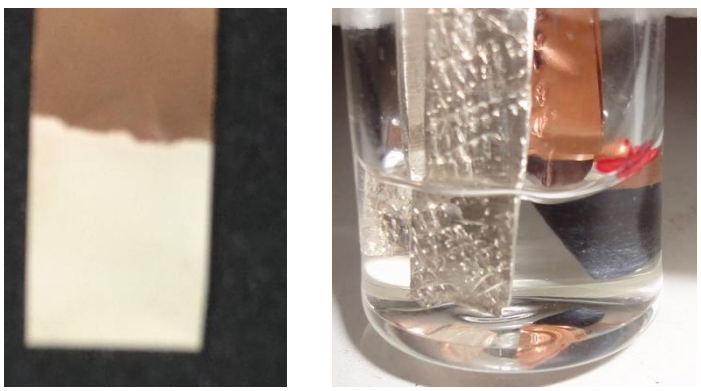

Figure S2 The naked white electrode turned into a black electrode after Li insertion.

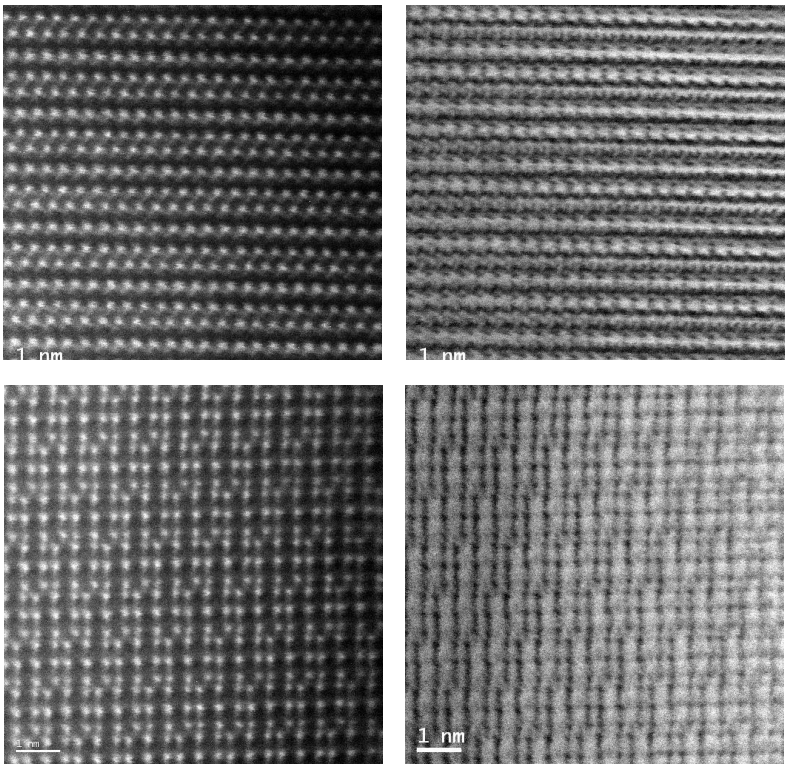

Figure S3: The HAADF (left) and ABF (right) images of $TiNb_2O_7$ at [$\bar{1}$10] zone axis (Up); the HAADF (left) and ABF (right) images of $TiNb_2O_7$ at [010] zone axis (Down).

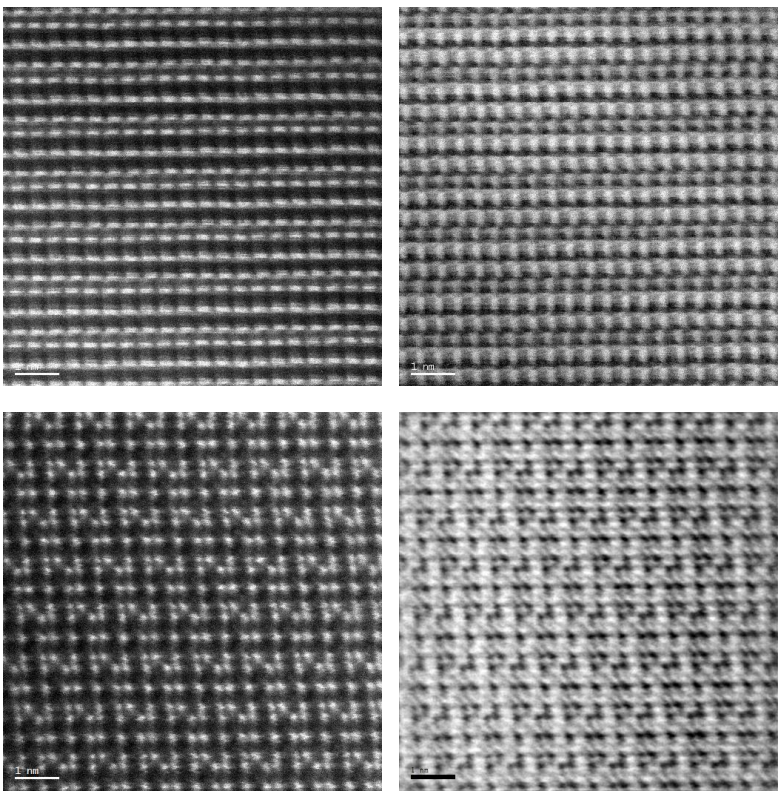

Figure S4: The HAADF (left) and ABF (right) images of $TiNb_2O_7$ discharged to 1.0 V at [$\bar{1}$10] zone axis (Up); the HAADF (left) and ABF (right) images of $TiNb_2O_7$ discharged to 1.0 V at [010] zone axis (Down).

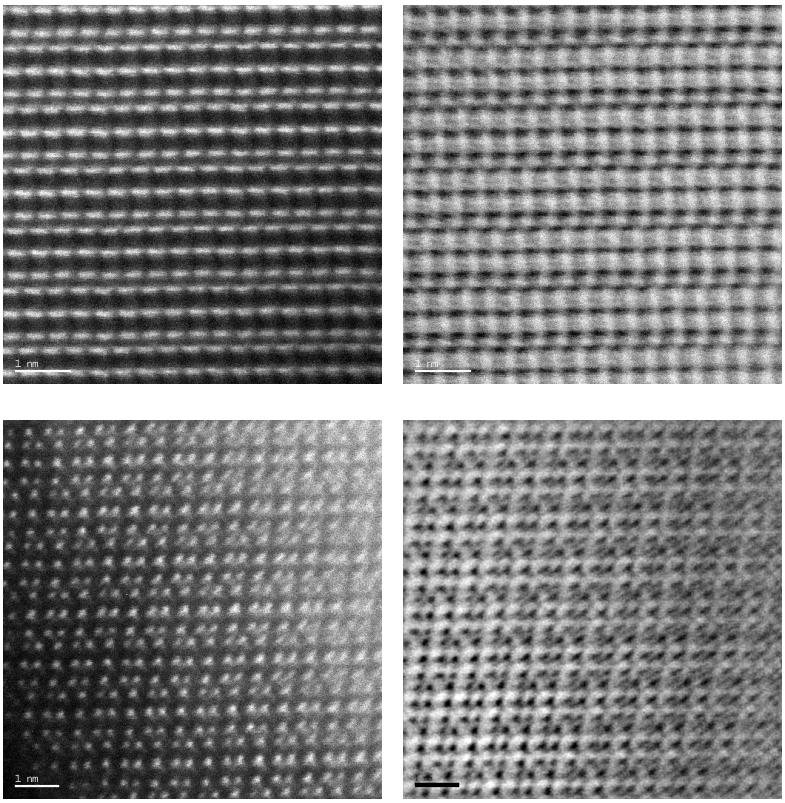

Figure S5: The HAADF (left) and ABF (right) images of $TiNb_2O_7$ charged to 3.0 V at [$\bar{1}$10] zone axis (Up); the HAADF (left) and ABF (right) images of $TiNb_2O_7$ charged to 3.0 V at [010] zone axis (Up)

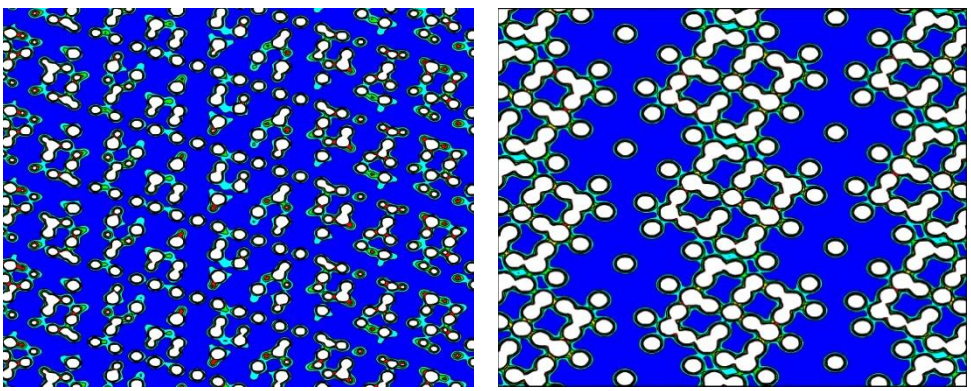

Figure S6: The (110) (left) and (001) (right) plane charge density of $TiNb_2O_7$.