

Supporting Information for

Towards understanding the effects of carbon and nitrogen-doped carbon coating on electrochemical performance of $\text{Li}_4\text{Ti}_5\text{O}_{12}$ in Lithium ion batteries: a combined experimental and theoretical study

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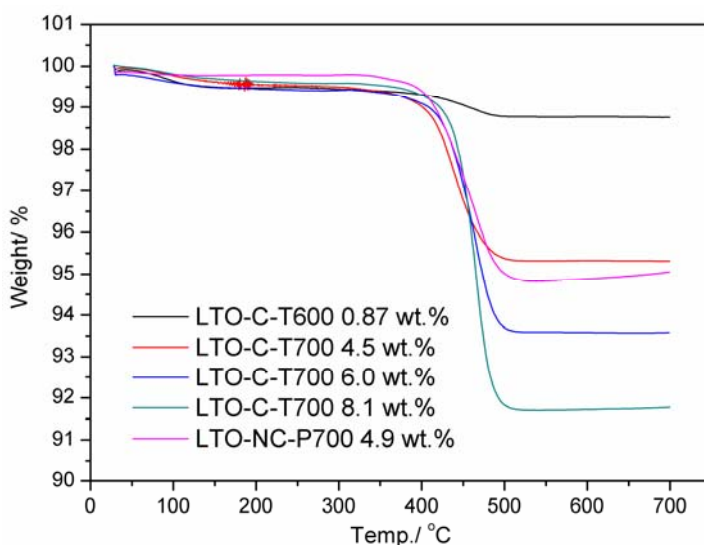


Figure S1 TG curves of carbon and N-doped carbon-coated LTO samples by a CVD method..

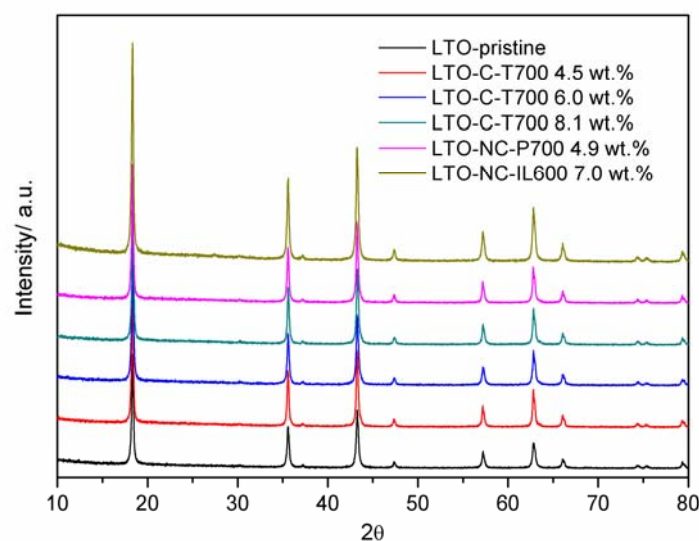


Figure S2 XRD patterns of carbon-coated LTO with different carbon contents.

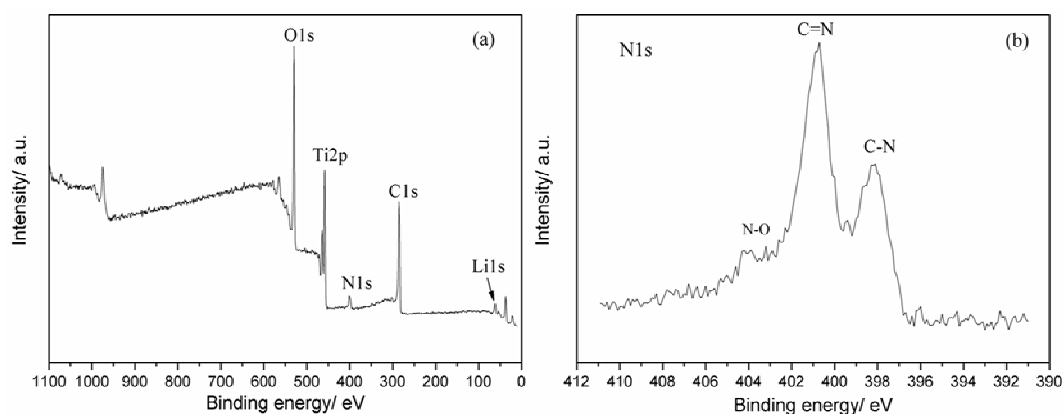


Figure S3 XPS survey spectrum of the LTO-NC-P700 sample (a) and its high resolution spectrum of N1s (b).

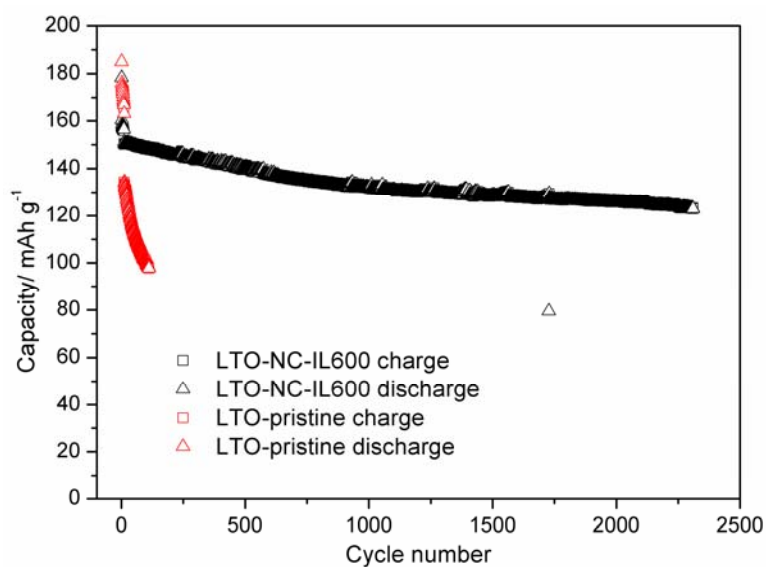


Figure S4 Cycling performance of N-doped carbon-coated LTO and pristine LTO.

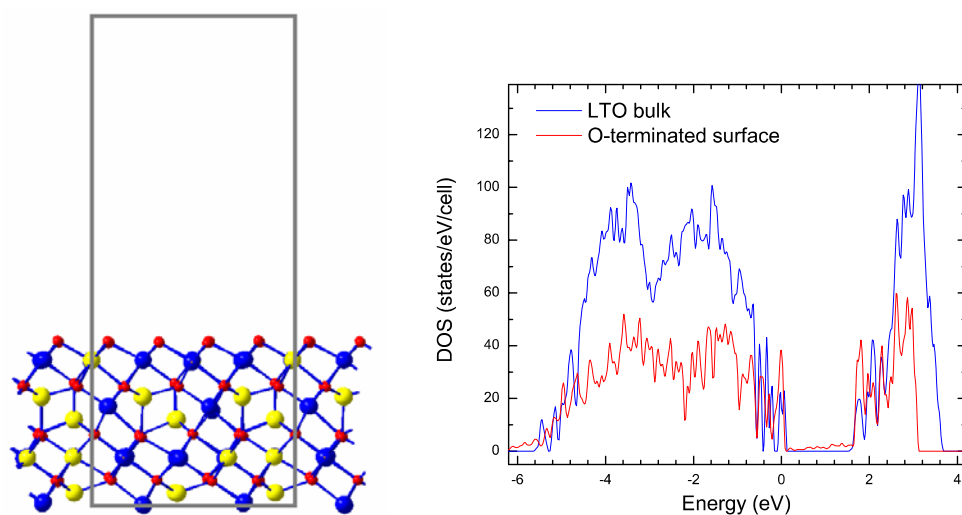
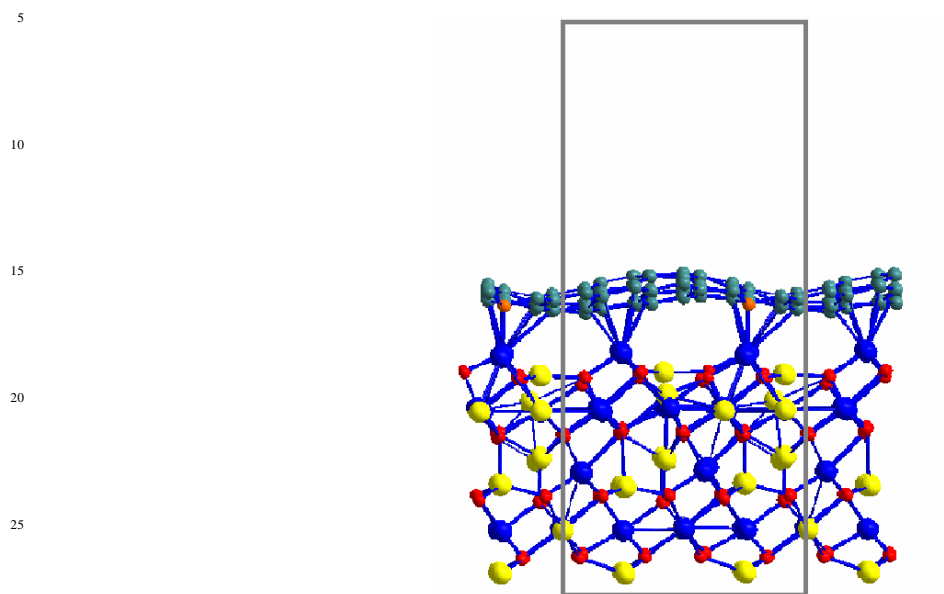


Figure S5 (Left) Atomic structure of O-terminated LTO(111) surface. (Right) Density of states (DOS) of bulk LTO (blue curve) and the DOS of O-terminated LTO (111) surface. The Fermi level is set to zero.



30 Figure S6 Side view of an N doped (3.2 wt.%) graphene-coating layer adsorbed on the Ti-terminated LTO surface. The gray rectangle represents the unitcell used in the calculations.