Supporting Information

Ultrathin TiO_2-B Nanowires as Anode Material for Mg-Ion Batteries Based on a Surface Mg Storage Mechanism

Yuan Meng[a], Dashuai Wang[a], Yingying Zhao[a], Ruqian Lian[a], Yingjin Wei[a,*], Xiaofei Bian[a], Yu Gao[a,*], Fei Du[a,b], Bingbing Liu[b], Gang Chen[a,b]

[a]Key Laboratory of Physics and Technology for Advanced Batteries (Ministry of Education), College of Physics, Jilin University, Changchun 130012, P. R. China.

[b]State Key Laboratory of Superhard Materials, Jilin University, Changchun 130012, P. R. China.

Corresponding author: yjwei@jlu.edu.cn (Y. J. Wei), yugao@jlu.edu.cn (Y. Gao);

Tel & Fax: 86-431-85155126.

Experimental

Preparation of the TiO_2-B reference sample: 0.4 g commercial TiO_2 (P25, Degussa) was dispersed in 40 ml 10 M NaOH under magnetic stirring and ultrasonic treatment. The resulting suspension was transferred into a 50 ml Teflon autoclave and subjected to hydrothermal treatment at 170 ^oC for 60 h. After cooling to room temperature, a white precipitate was collected by centrifugation and washed with de-ionized water and dilute hydrochloric acid. This intermediate product was constantly stirred in 0.1 M HCl for 8 h to complete the H^+/Na^+ exchange reaction. Then the material was frozen-dried at -30 ^oC for 20 h. Finally, a white powder was collected and heat treated at 400 ^oC for 4 h in air to get the TiO_2-B nanowires.

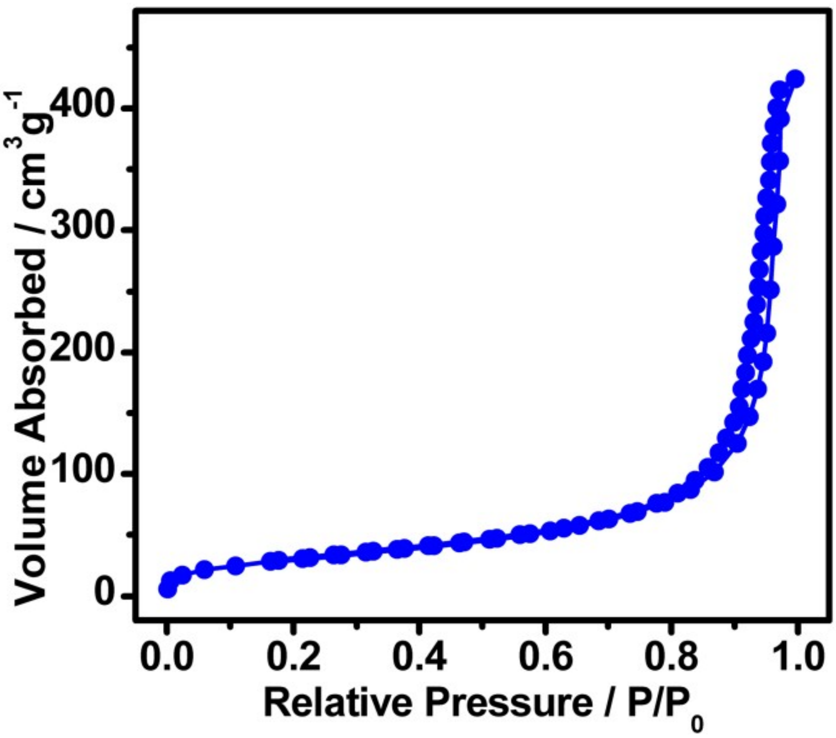

Figure S1. Nitrogen adsorption-desorption isotherms of the TiO_2-B nanowires.

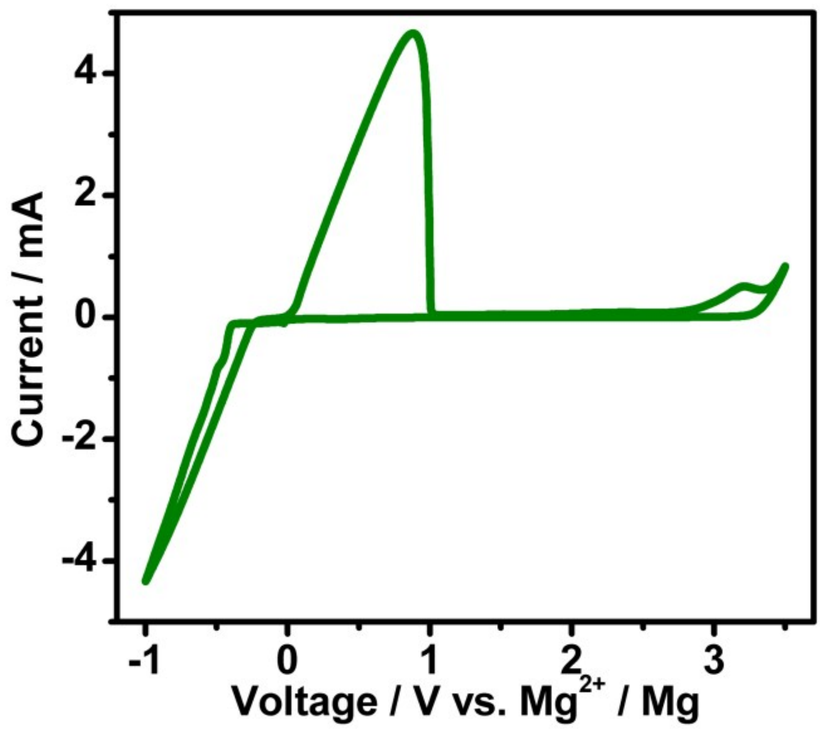

Figure S2. CV curve from the three-electrode cell using the APC/THF electrolyte, Pt as the working electrode and Mg as the reference and counter electrodes.

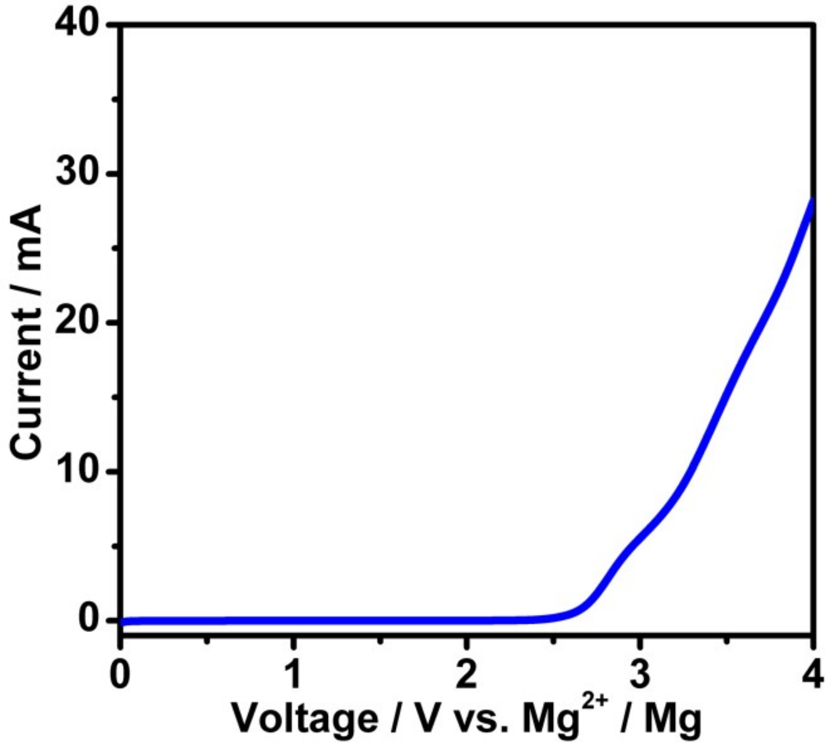

Figure S3. LSV curve obtained from a coin cell using the APC/THF electrolyte, SSF as the working electrode and Mg as the counter electrode.

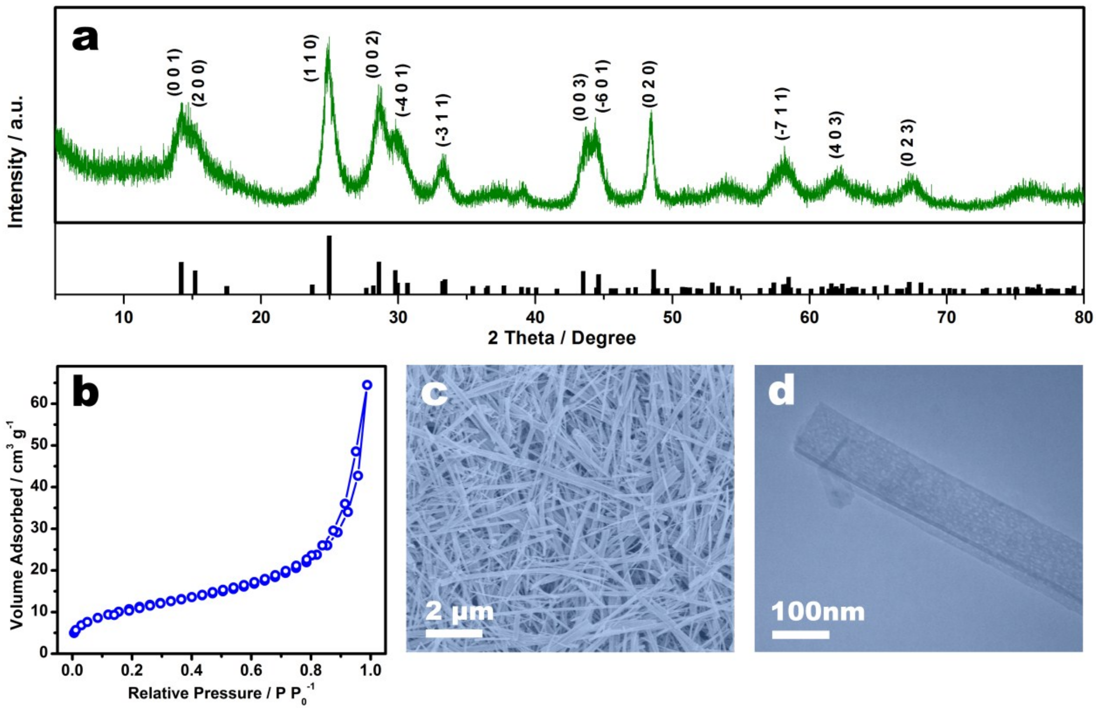

Figure S4. XRD (a), N_2 adsorption-desorption isotherms (b), SEM (c) and TEM (d) of the reference TiO_2-B nanowire sample.

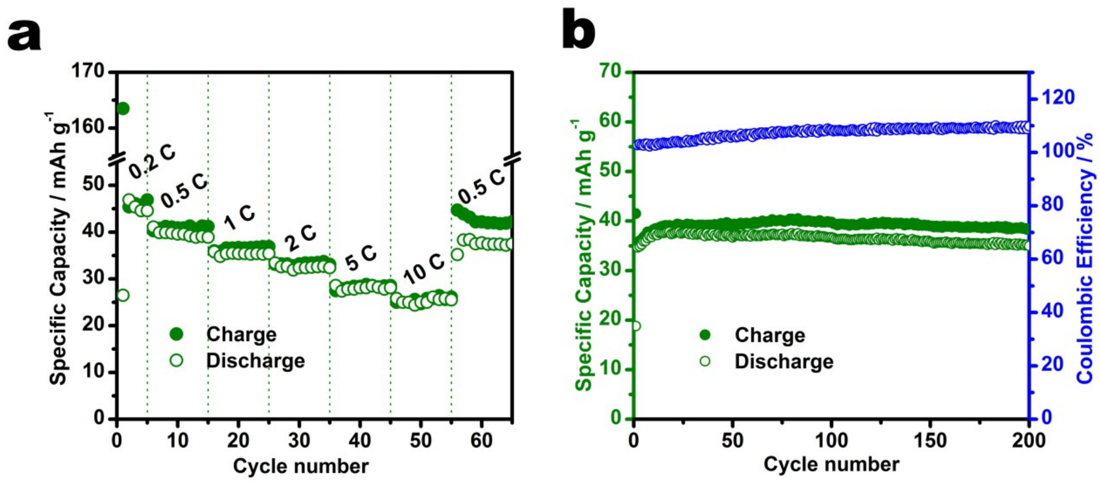

Figure S5. Rate performance (a) and charge-discharge cycling performance at 2C rate (b) for the reference TiO_2-B nanowire sample.

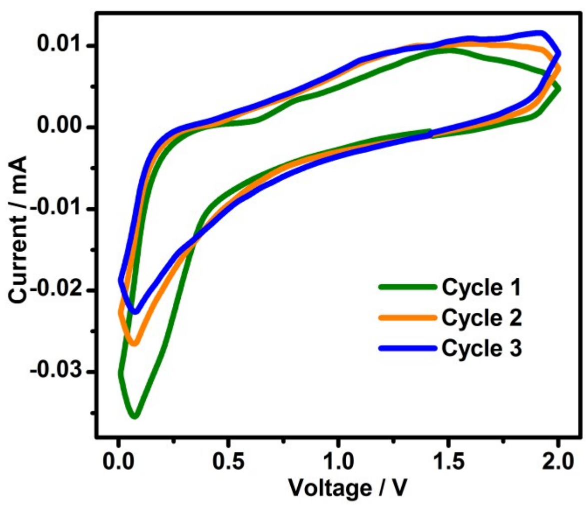

Figure S6. CV curves of the TiO_2-B nanowires at a scanning rate of 0.05 $mV{\cdot}s^{-1}$.

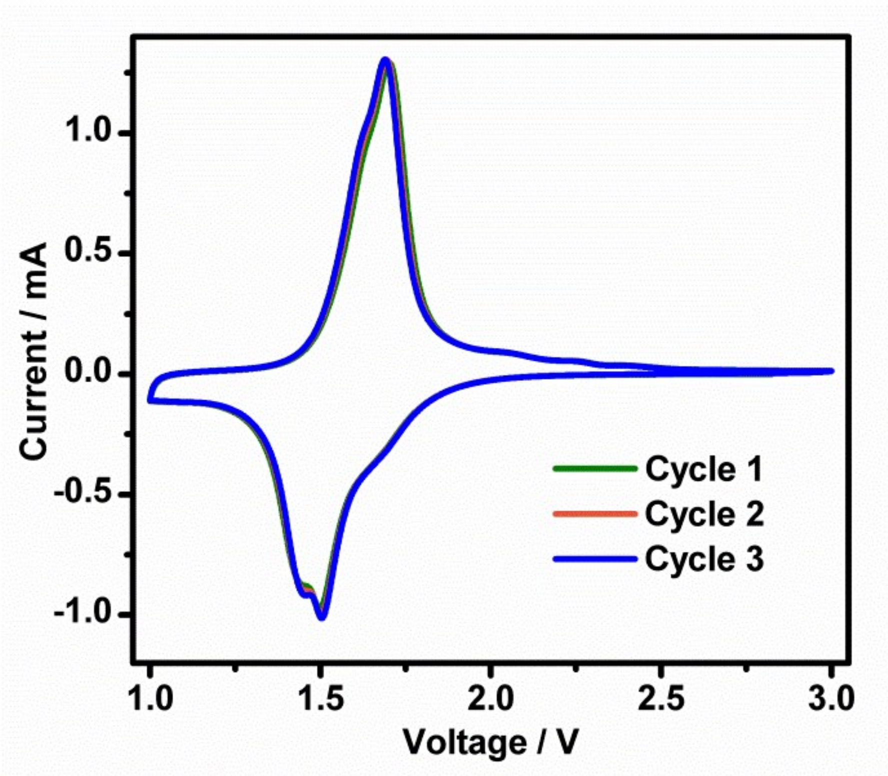

Figure S7. CV of the TiO_2-B nanowires in a 1.0 M $LiPF_6$ electrolyte dissolved in ethylene carbonate (EC) and dimethyl carbonate (DMC) (EC : DMC = 3 : 7).

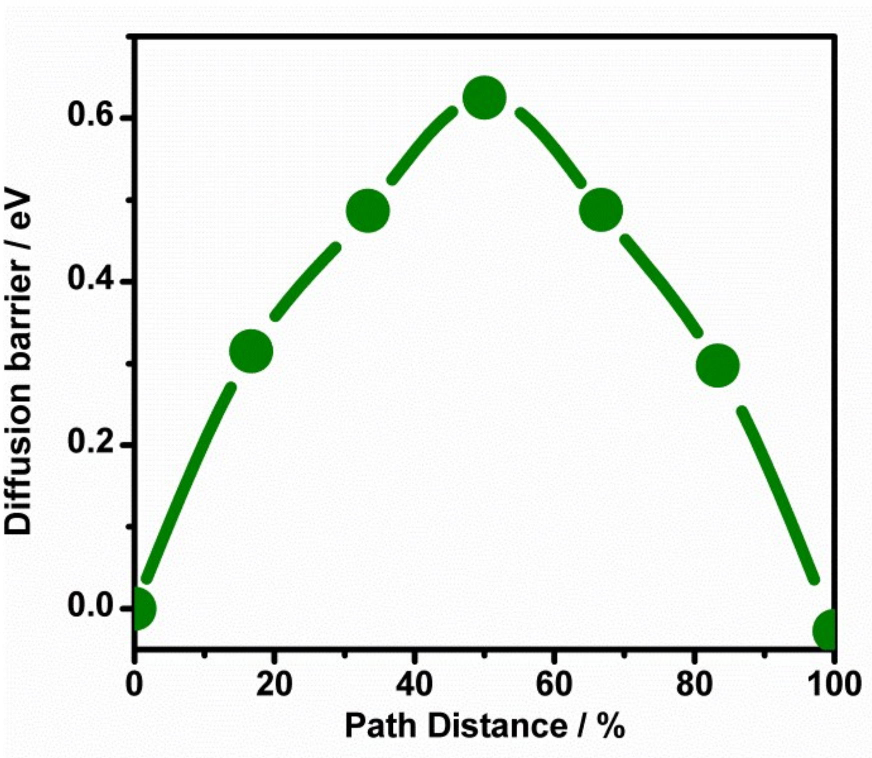

Figure S8. Calculated diffusion barrier for Mg^{2+} ions in TiO_2-B.

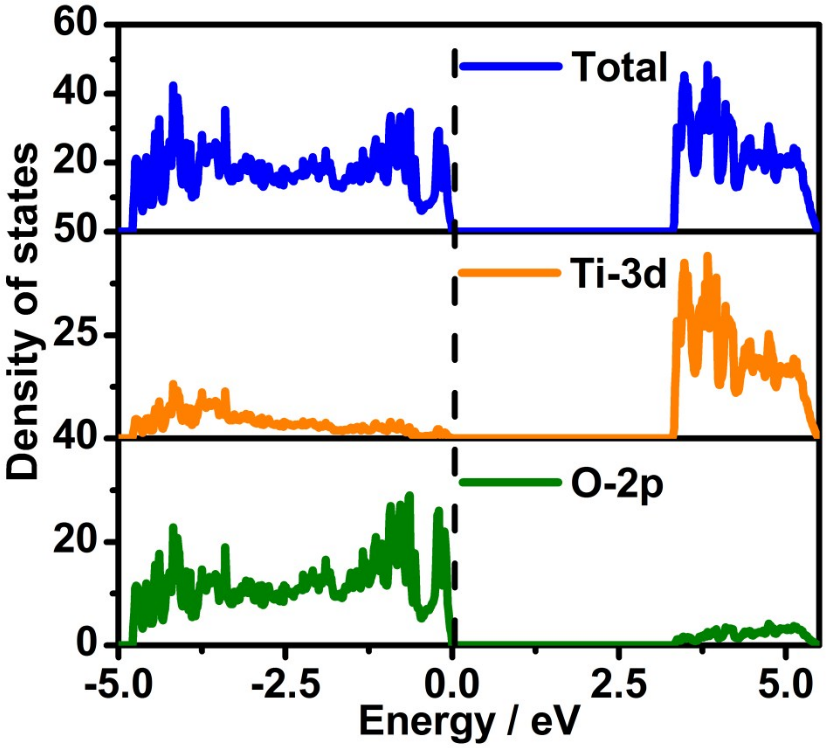

Figure S9. Total and projected density states of TiO_2-B.

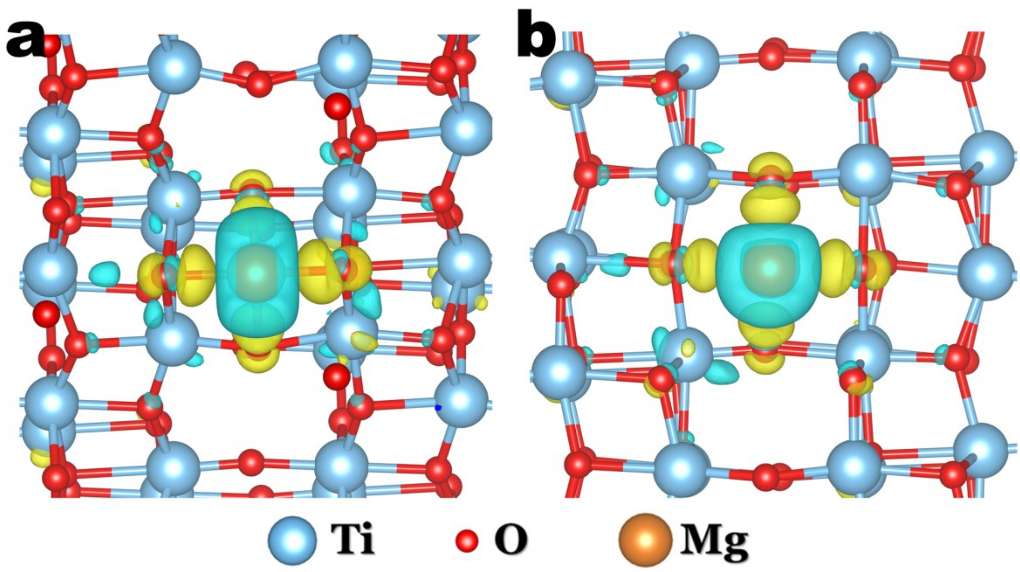

Figure S10. The charge difference isosurfaces of Mg^{2+} ion adsorption on the site A2 (left) and C (right) sites of TiO_2-B (-110) surface, respectively; isosurface level is set to 0.005 e/Å^3.

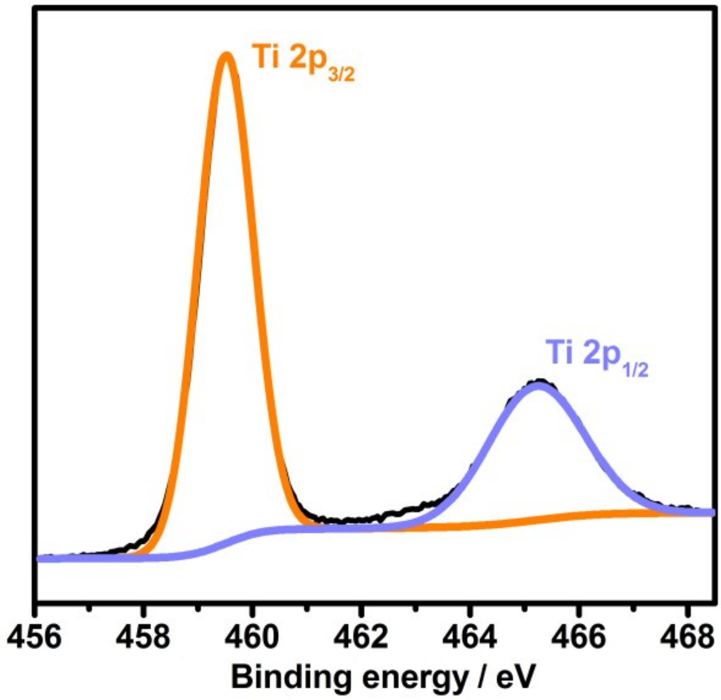

Figure S11. Ti *2p* XPS pattern of the TiO_2-B nanowires.

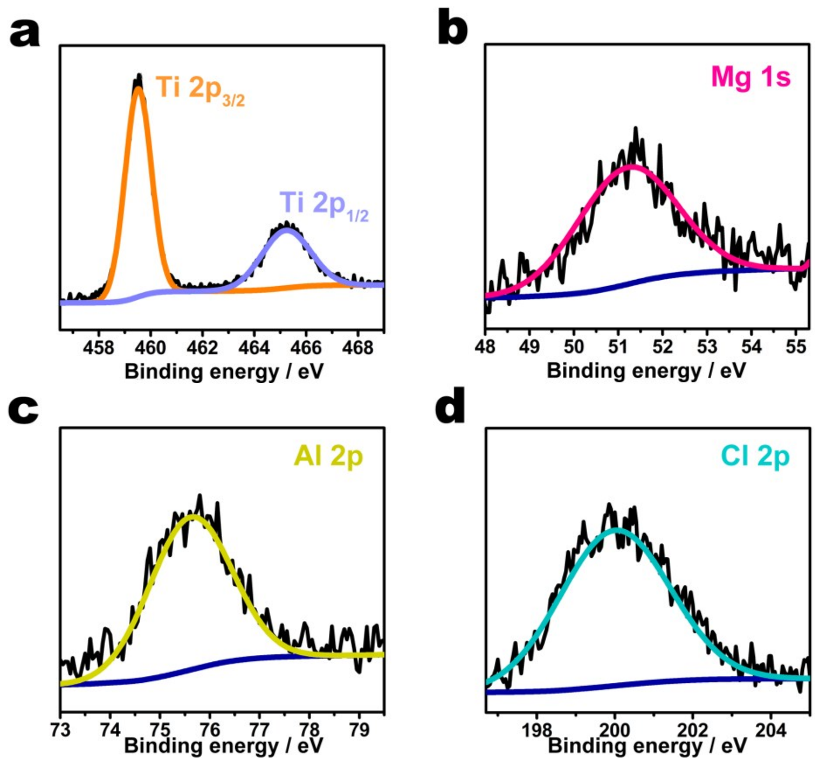

Figure S12. (a) Ti *2p*, (b) Mg *1s*, (c) Al *2p*, and (d) Cl *2p* XPS patterns of the TiO_2-B electrode held at the open-circuit voltage (OCV) for 36 h.

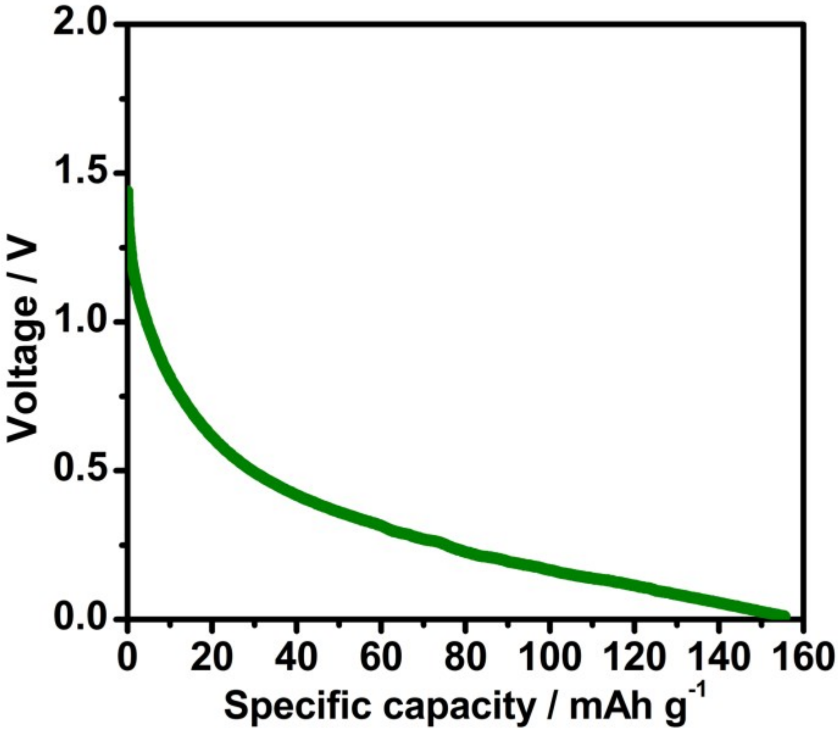

Figure S13. First discharge curve of the TiO_2-B nanowires in Mg ion batteries.