Electronic Supplementary Information

High-rate lithium storage of anatase TiO_2 crystals doped with both nitrogen and sulfur

Sample preparation Anatase TiO_2 nanoparticles used in this work were prepared according to the procedures by Chen *et al*. [22]. These anatase TiO_2 nanoparticles were heated at 700 ^oC for 18 h in gaseous ammonia atmosphere with a flux of 100 mL/min to prepare TiN_x. The resultant TiN_x was then oxidized at 340 ^oC in static air for 2 h to obtain nitrogen doped TiO_2 (N-TiO_2). Sulfur codoping was realized by treating N-TiO_2 at 400 ^oC in gaseous H_2S atmosphere with a flux of 50 mL/min for 1 h (N/S-TiO_2). S doped TiO_2 reference (S-TiO_2) was prepared by treating anatase TiO_2 nanoparticles at 400 ^oC in gaseous H_2S atmosphere with a flux of 50 mL/min for 1 h.

Characterization X-ray diffraction (XRD) patterns of the samples were recorded on a Rigaku diffractometer using Cu Kα irradiation. Their morphology was determined by transmission electron microscopy (TEM) performed on JEOL2010 electron microscope. The Brunauer-Emmett-Teller (BET) specific surface area and pore size was determined by nitrogen adsorption-desorption isotherm measurements at 77 K (ASAP 2010). The chemical states of dopants in TiO_2 were analyzed using X-ray photoelectron spectroscopy (Thermo Escalab 250, a monochromatic Al Kα X-ray source). Binding energy was referenced to the C 1s peak (284.6 eV) arising from adventitious carbon. The optical absorbance spectra of the samples were recorded in a UV-visible spectrophotometer (JASCO-550).

Electrochemical measurements The electrochemical properties of TiO_2, N-TiO_2,

N/S-TiO_2 as anode materials in lithium ion batteries were evaluated by a galvanostatic charge/discharge technique. The working electrodes were prepared by mixing the active material, carbon black (Super-P), and poly(vinyl difluoride) at a weight ratio of 80:10:10 and pasted onto pure aluminium foil, and pressed and dried under vacuum at 120 ^{o}C for 12 h. Coin cells were assembled in an argon-filled glove box, with metallic lithium as the counter electrode, 1 M $LiPF_6$ in ethylene carbonate, dimethyl carbonate (1:1 vol) as electrolyte, and Celgard 2400 polypropylene as separator. The electrochemical tests were performed between 1-3 V vs. Li^+/Li. C-rate currents used were calculated based on an anatase TiO_2 theoretical capacity of 168 mA hg^{-1}.

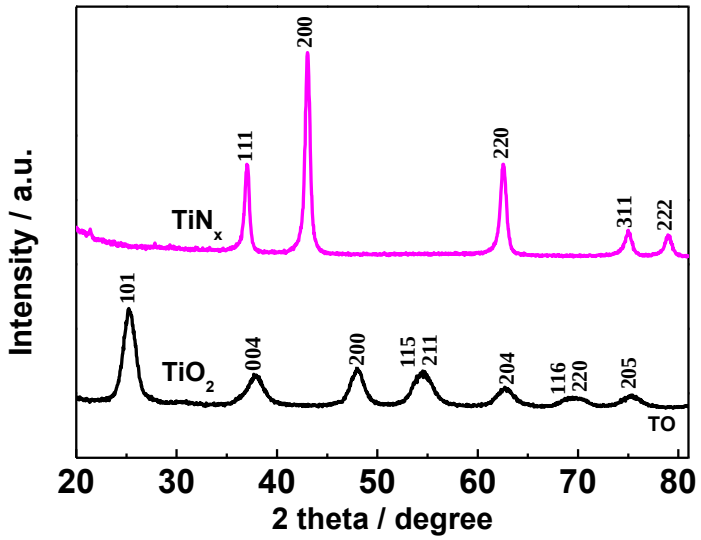

Fig. S1 XRD patterns of TiO_2 and TiN_x.

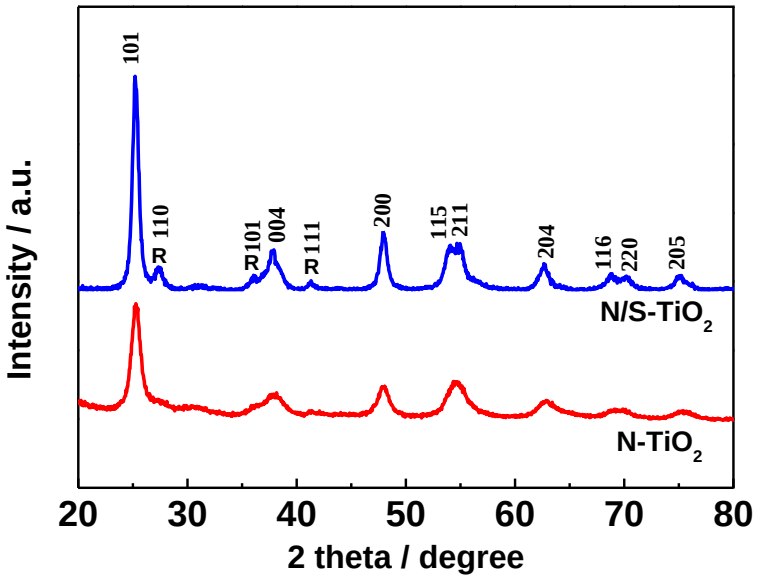

Fig. S2 XRD patterns of N-TiO_2 and N/S-TiO_2. R: rutile.

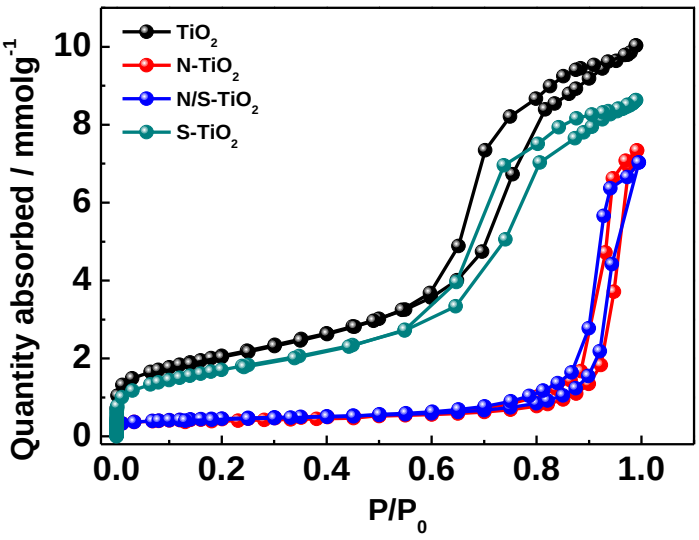

Fig. S3 N_2 isotherm adsorption-desorption curves of TiO_2, N-TiO_2, S-$TiO_2$and N/S-TiO_2.

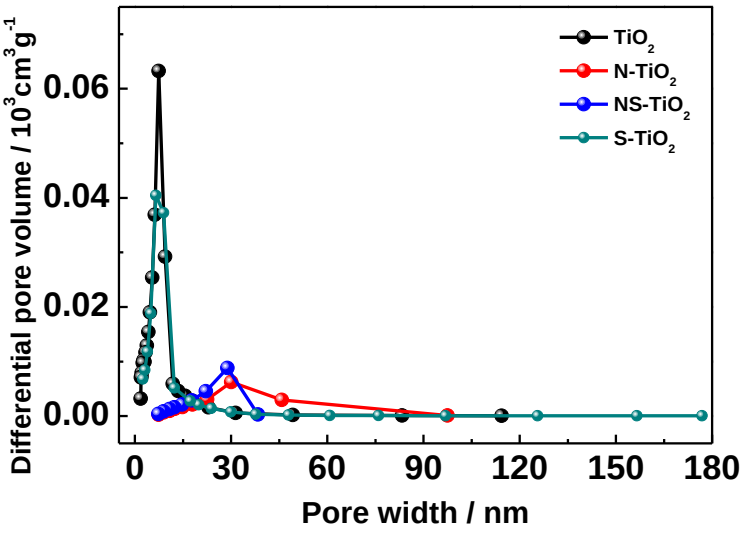

Fig. S4 Pore size distribution curves of TiO_2, N-TiO_2, S-TiO_2 and N/S-TiO_2.

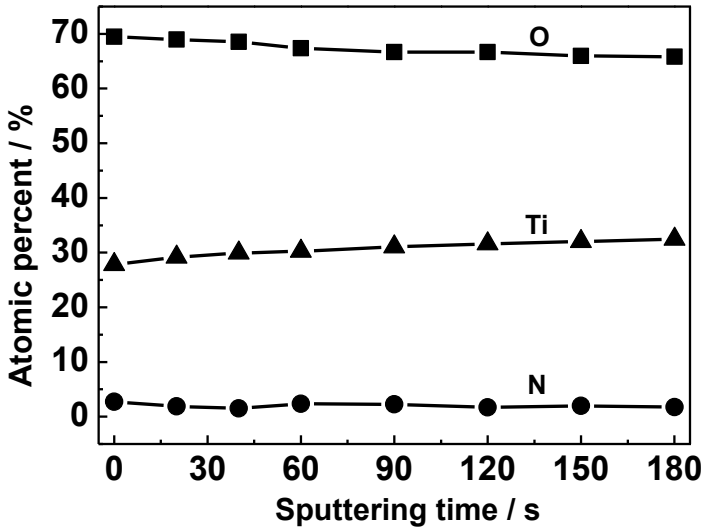

Fig. S5 XPS depth profiles of the elements of Ti, O and N in N-TiO_2 upon Ar^+ sputtering.

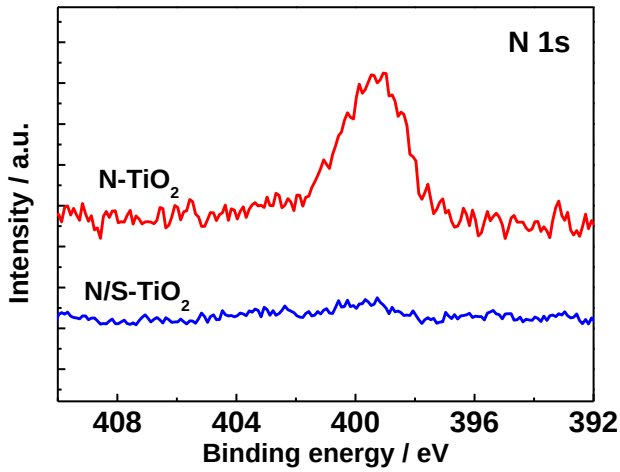

Fig. S6 High resolution N 1s XPS spectra recorded from the pristine surface of N-TiO_2 and N/S-TiO_2.

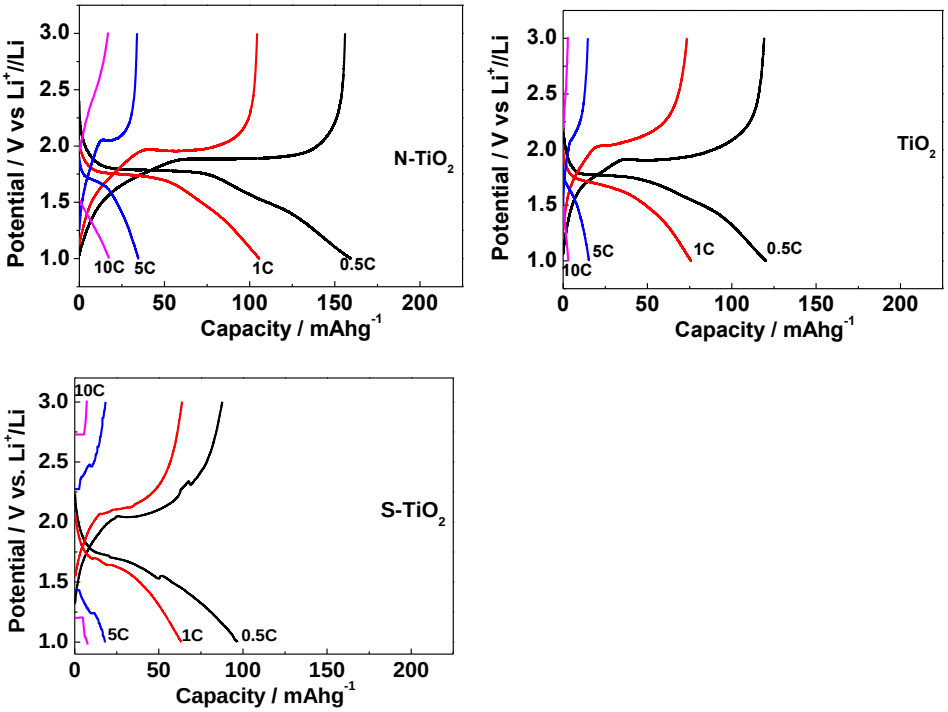

Fig. S7 Galvanostatic charging/discharging curves of the N-TiO_2, S-TiO_2 and TiO_2 electrodes at different rates.

Table S1 Impedance parameters calculated from equivalent circuits.

Materials	R_e (Ω)	R_{ct} (Ω)
TiO_2	13.7	282.0
N-TiO_2	11.2	181.6
S-TiO_2	11.4	248.3
N/S-TiO_2	9.4	89.6