Supporting Information

Nanoporous hexagonal TiO_2 superstructure as a multifunctional material for energy conversion and storage

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KEYWORDS. Hexagonal TiO_2 superstructure, grain growth mechanism, nano-pores, dye-sensitized solar cells, lithium ion batteries

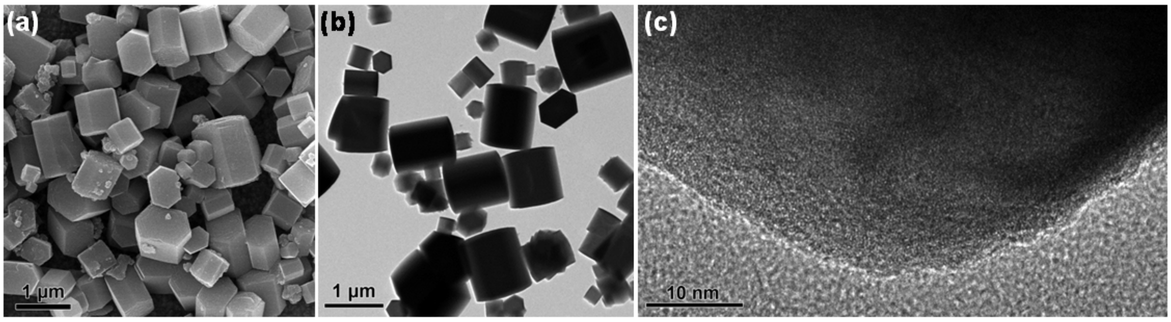


Fig. S1 (a) SEM and (b and c) TEM images of HTO.

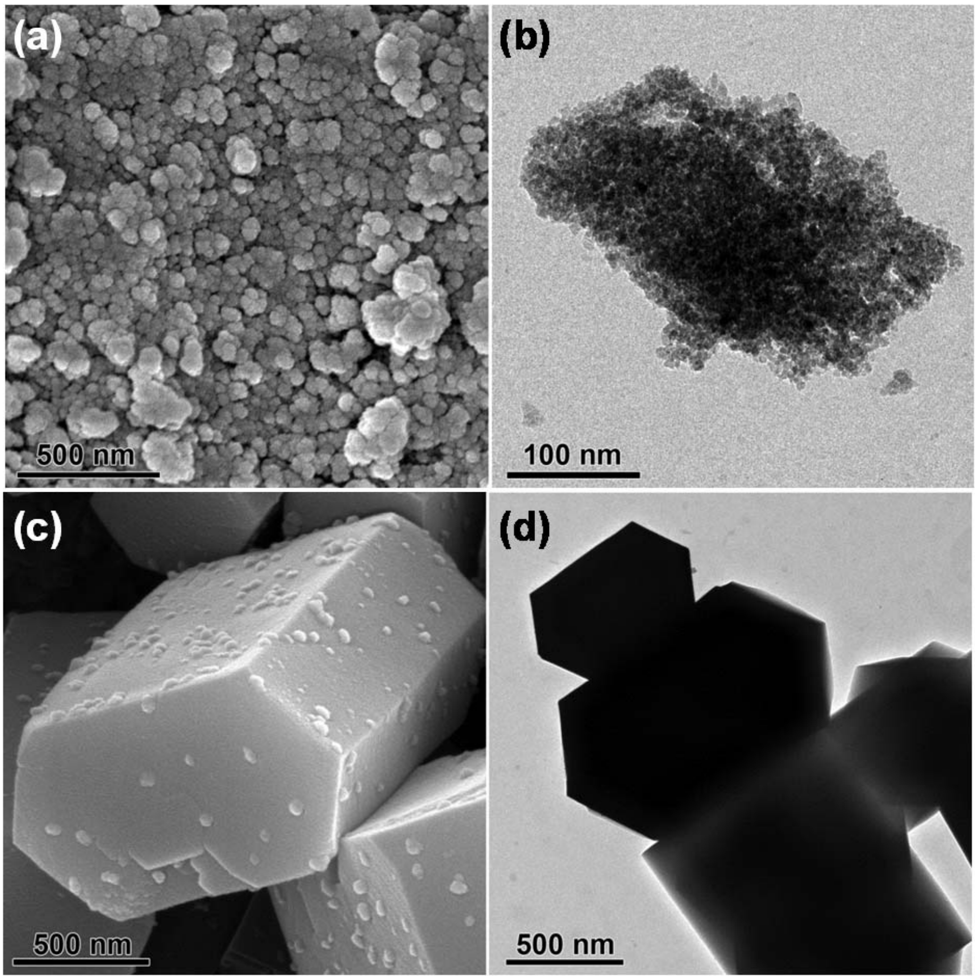


Fig. S2 (a) SEM and (b) TEM images of TiO_2 precursor prepared without oxalic acid (OA) and (c) SEM and (d) TEM images of TiO_2 precursor prepared without sodium dodecyl benzene sulfonate (SBDS).

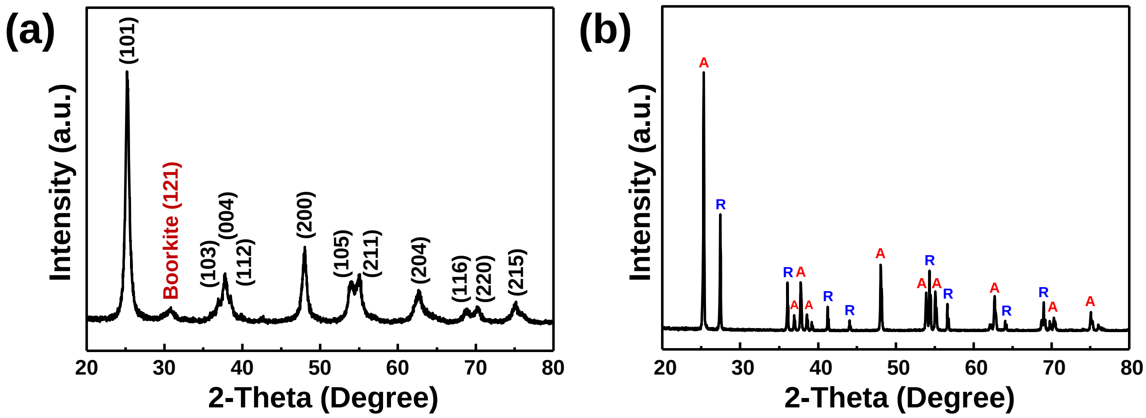


Fig. S3 XRD pattern of (a) anatase/brookite TiO_2 obtained when HTO powder was directly transferred to a furnace held at 450 °C and annealed for 5 h and (b) anatase/rutile TiO_2 obtained when HTO powder was annealed at 900 °C for 5 h.

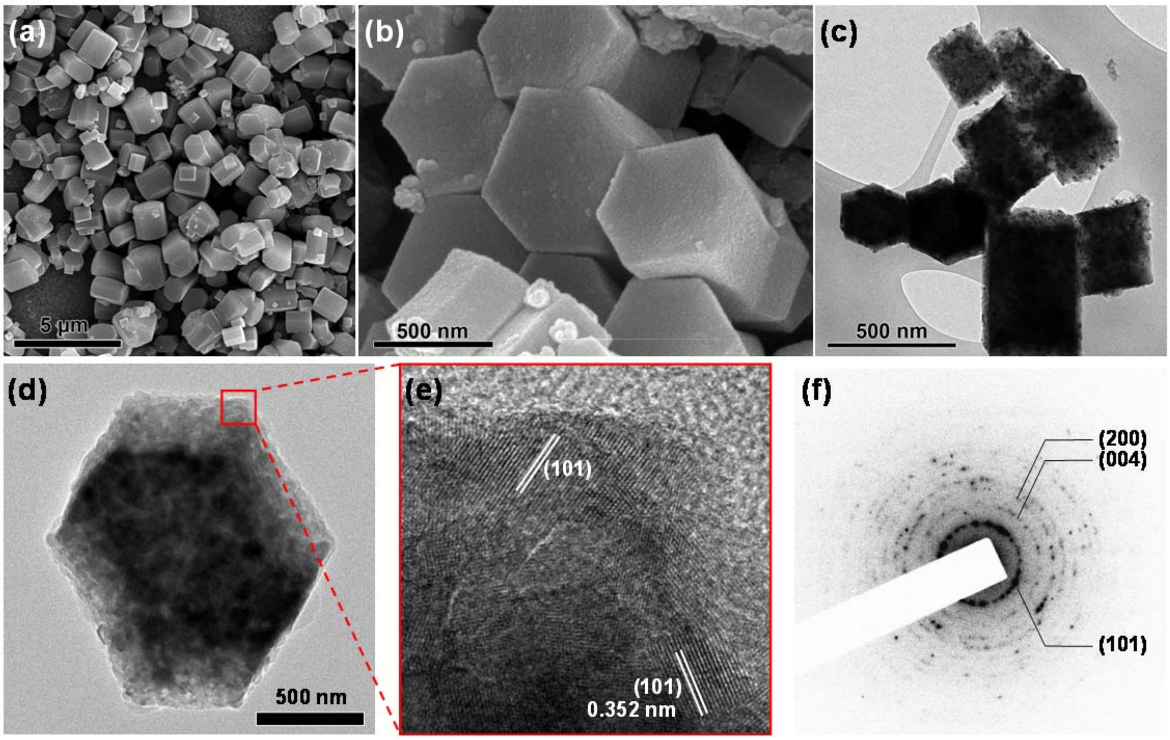


Fig. S4 (a and b) SEM and (c-e) TEM images of HTS obtained by calcining HTO, and (f) its selected-area electron diffraction (SAED) patterns.

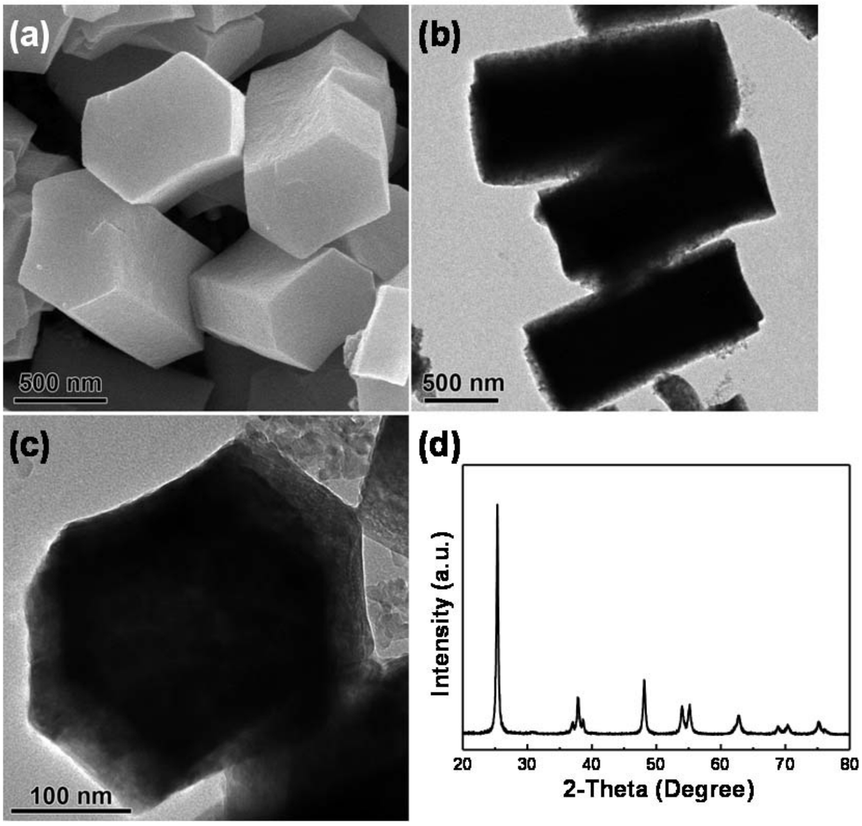


Fig. S5 (a) SEM and (b) TEM images of TiO_2 obtained by calcining the TiO_2 precursor prepared without sodium dodecyl benzene sulfonate (SBDS), (c) XRD pattern of TiO_2 obtained by calcining the TiO_2 precursor prepared without sodium dodecyl benzene sulfonate (SBDS).

Table S1. Solar Cell Parameters of DSSCs with Various TiO_2 Films.

TiO_2 films	J_{sc} (mA cm^{-2})	V_{oc} (V)	FF	η (%)
NT/HTS	18.0	0.74	0.57	7.6
NT only	16.0	0.73	0.56	6.4
NT/DSL	16.7	0.73	0.56	6.8

Table S2. Solar Cell Parameters of DSSCs with TiO_2 Film of NT/HTS from multiple cell measurements.

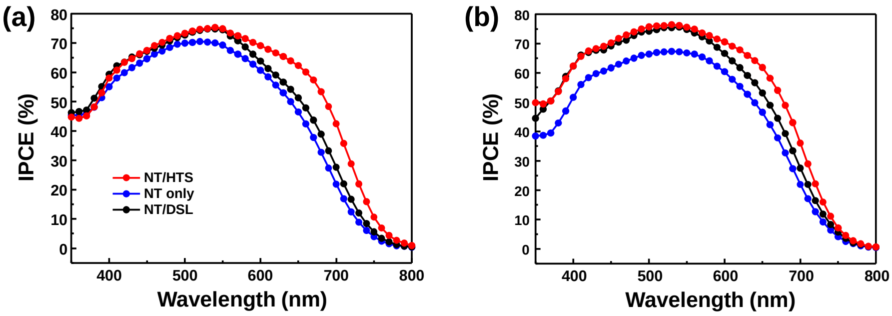
NT/HTS	Jsc (mA/cm^2)	Voc (V)	FF	Eff (%)
Cell 1	18.0	0.737	0.570	**7.58**
Cell 2	18.2	0.741	0.555	7.48
Cell 3	17.6	0.737	0.575	7.44

Table S3. Solar Cell Parameters of DSSCs with TiO_2 Film of NT only from multiple cell measurements.

NT only	Jsc (mA/cm^2)	Voc (V)	FF	Eff (%)
Cell 1	16.0	0.732	0.558	**6.44**
Cell 2	16.1	0.722	0.570	6.61
Cell 3	15.9	0.707	0.565	6.33

Table S4. Solar Cell Parameters of DSSCs with TiO_2 Film of NT/DSL from multiple cell measurements.

NT/DSL	Jsc (mA/cm^2)	Voc (V)	FF	Eff (%)
Cell 1	16.7	0.725	0.562	**6.81**
Cell 2	16.5	0.725	0.567	6.79
Cell 3	16.3	0.731	0.584	6.94



Solar Cell	J_{sc} (mA/cm^2)
NT/HTS	14.34
NT only	12.11
NT/DSL	13.04

Solar Cell	J_{sc} (mA/cm^2)
NT/HTS	14.30
NT only	11.76
NT/DSL	13.38

Fig. S6 IPCE curves of DSSCs with different photoanodes from multiple measurements and photocurrent obtained by integration of IPCE spectra. Note that the integrated J_{sc} values from the IPCE measurements are lower than those from *J-V* curve measurement because of mismatch in area and shape between excitation beam (rectangle: 0.1 cm×0.7 cm) and active area of solar cells (circle with 0.5 cm in diameter). Thus, some of photons from the excitation did not reach the active area during IPCE measurements.

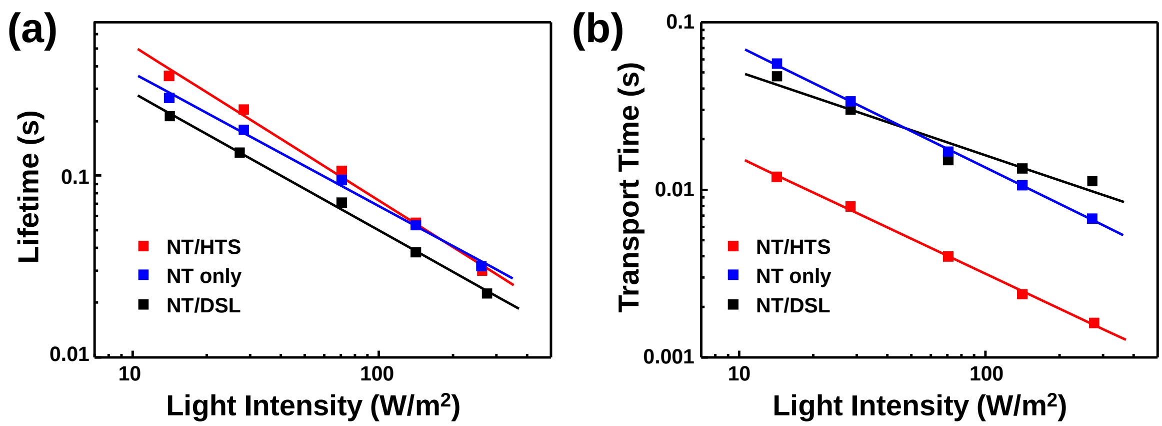


Fig. S7 (a) Electron lifetime and (b) electron transport time as a function of light intensity for DSSCs with different TiO_2 layers.

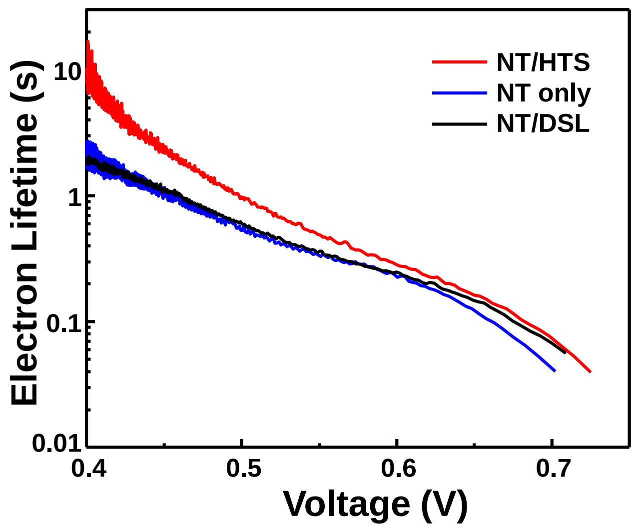


Fig. S8 Electron lifetimes of DSSCs with different TiO_2 layers obtained from photovoltage decay measurement.

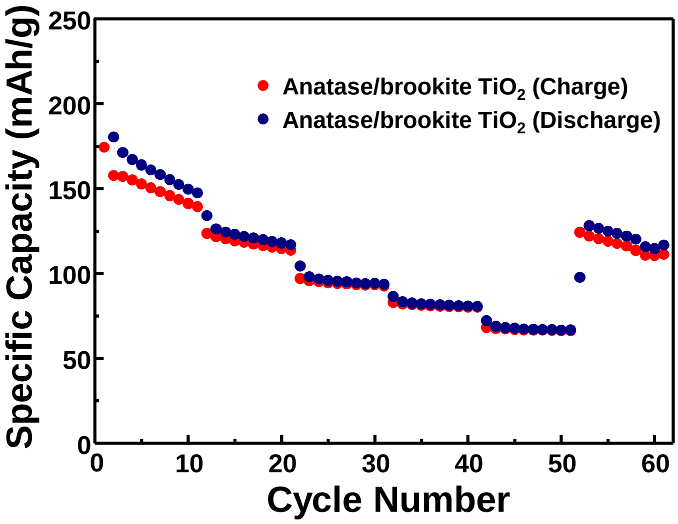


Fig. S9 Specific capacities of anatase/brookite TiO_2 at various C rates.

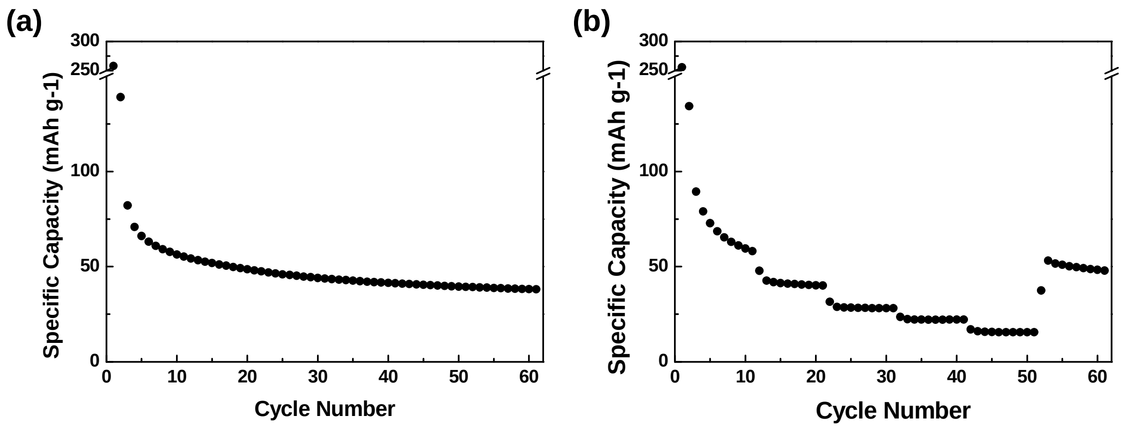


Fig. S10 (a) Specific capacities of P25 anodes at 0.5 C during the first 100 galvanostatic cycles and (b) specific capacities of P25 cycled at various C-rates (0.5, 1, 2, 3, 5, and 0.5 C).

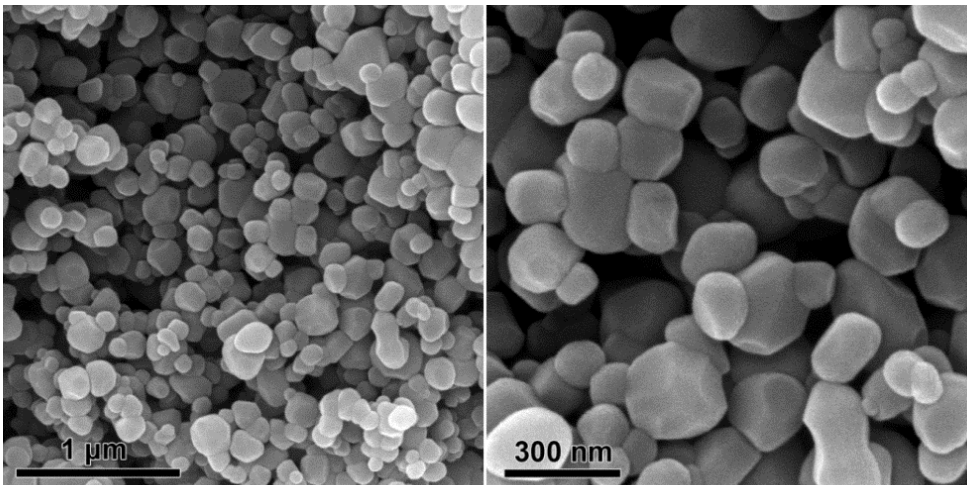


Fig. S11 SEM images of C-TiO_2 (anatase, Sigma-Aldrich).

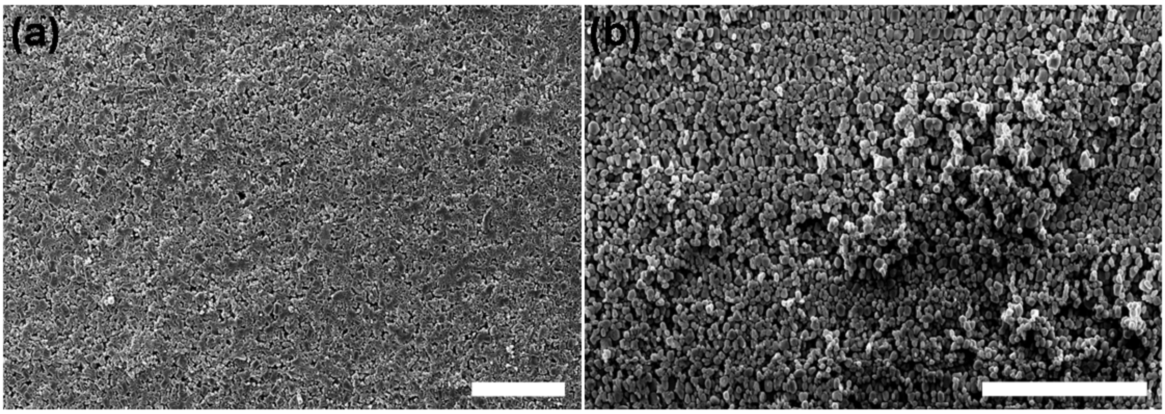


Fig. S12 SEM images of (a) pelletized HTS and (b) pelletized conventional anatase TiO_2 spheres. Scale bar is 10 μm.

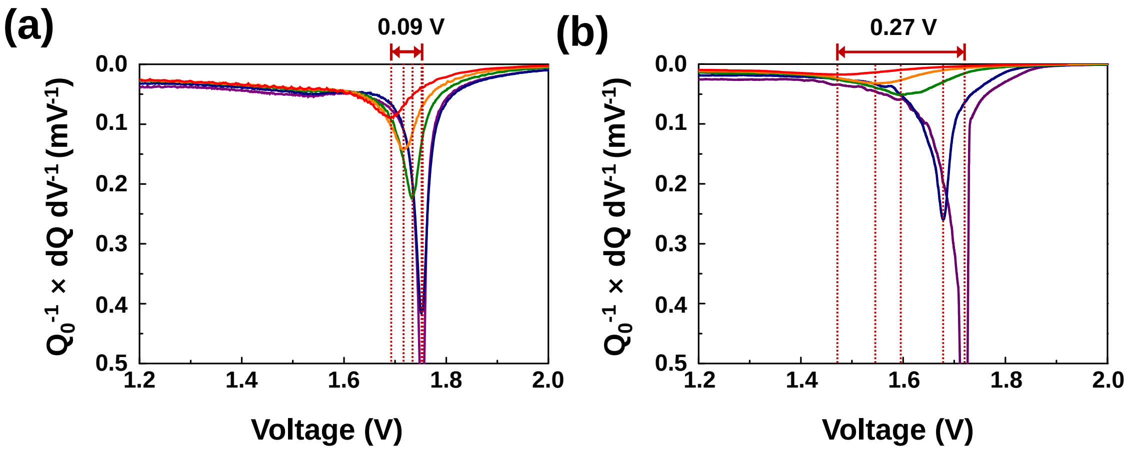


Fig. S13 Differential capacities of (a) HTS and (b) C-TiO_2 anodes at various C-rates.

Table S5. Fitted Impedance Parameters of Nyquist Plots.

Active material	R_s (Ω)	R_{ct} (Ω)	Q_y of CPE_{pn} (mF)	A_w* (mΩ $s^{-0.5}$)
HTS	3.29	119.1	42.6	0.4
C-TiO_2	4.19	246.4	0.9	28.7

*$A_w = RT/(n^2F^2A2^{1/2})(2/D^{1/2}C)$.

where R is the gas constant, T is the temperature, *n* is the transferred electron number, A is the electrode area, D is the diffusion coefficient of Li^+ in electrode and C is the concentration of Li^+.