Supplementary Information (SI) for Nanoscale.

Supporting Information

Rigid organic molecule pillared Ti_3C_2 towards high rate capability and fast sodium ion storage

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Material Characterization

Scanning electron microscope SEM (JSM-6701F) and transmission electron microscope TEM (JEM-2010) were used to analyze the micromorphology and structure of Ti_3C_2 and Ti_3C_2-BTCA. The chemical state of elements of samples was measured by XPS (AXIS-SUPRA). FTIR was tested to discover the appearance of a new chemical bond in Ti_3C_2-BTCA. The N_2 adsorption/desorption curves were tested by the surface area and pore size analyzer (JW-BK200). The XRD patterns were investigated by a Rigaku D/MAX 2400 diffractometer with Cu-Kα radiation (λ = 0.154 nm), and the calculation of interlayer spacing was done using the Bragg equation[1]：

$$d = \frac{\lambda}{2sin\theta_{(002)}} \qquad S\mathbf{1}$$

Electrochemical Measurement

Ti_3C_2-BTCA and other comparable active substances, Super P and PVDF binders were uniformly applied to copper foils at a ratio of 8:1:0.5, and half cells were assembled in an Ar atmosphere glove box.

Sodium-ion half-cells were assembled using sodium metal as the counter-electrode, copper foil coated with active substance as the working electrode, a Whatman GF/D type membrane and an organic electrolyte of 1.0 M $NaPF_6$ (EC:DC:DMC=1:1:1); The sodium metal electrode was also replaced by aluminium foil coated with activated carbon as the anode and the above electrode material as the cathode to form the sodium ion capacitor. The electrochemical data were tested using a LAND, CT2001 A and an electrochemical workstation (CHI660D) and the impedance was tested using an AUTOLAB AC impedance meter (PGSTAT T100N).

All the formulas you need to use in the article:

The relationship between the peak current (i) at the redox peak and the sweep rate was used to investigate the storage of sodium ions:

$$i = a \cdot v^b \qquad S2$$

where a and b are available and b depends on the slope of S3:

$$\log(i) = b \cdot log(v) + log(a) \qquad S3$$

When the b value is close to 1.0, it indicates surface capacitance control behavior, and when the b value is close to 0.5, it represents diffusion control capacitance behavior[2].

The diffusion contribution and the percentage of capacitance can be calculated according to the following equations:

$$i = k_1 v + k_2 v^{1/2} \qquad S4$$

Here k_1 and k_2 are constants, k_1v denotes the surface control capacitance and $k_2v^{1/2}$ denotes the diffusion control capacitance contribution[3].

From the constant current intermittent titration technique (GITT), the sodium ion diffusion coefficient was calculated according to the following equation:

$$D_{ions} = \frac{4l^2}{\pi\tau}\left(\frac{\Delta E_s}{\Delta E_t}\right)^2 \qquad \textbf{S5}$$

where L is the thickness of the ions through the electrode material, τ is the chirp time, ΔEs is the pulse induced voltage drop and ΔEt is the voltage difference during constant current charging/discharging[4].

Specific capacitance formula for sodium ion capacitors:

$$C_m = \frac{I \cdot \Delta t}{m \cdot \Delta v} \qquad S6$$

Formula to calculate the energy density.

$$E = \frac{1}{2} C_m \cdot \Delta t^2 \qquad S7$$

Power density calculation:

$$P = \frac{E}{\Delta t} \qquad S8$$

Where I(A) is the discharge current, Δt(s) is the discharge time, m(g) is the mass of the total active material at the positive and negative electrodes, and Δv(V) is the potential difference[5].

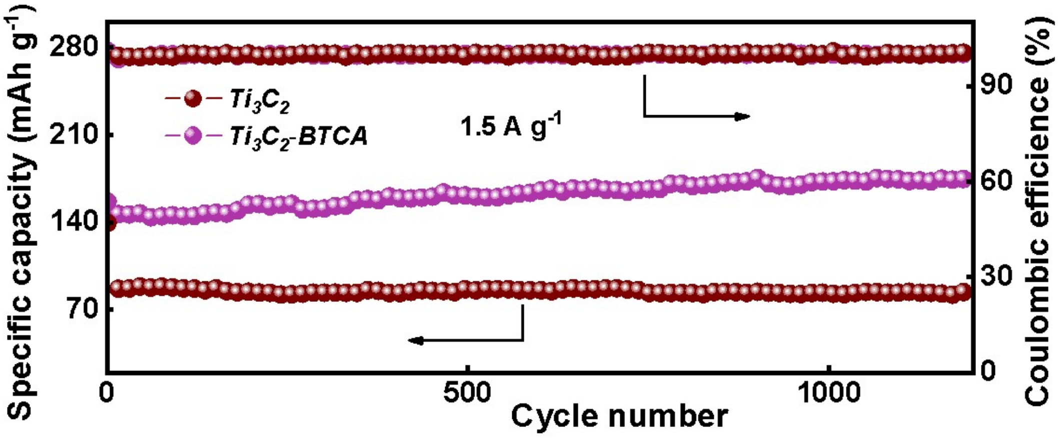

Figure S1. Cycle stability of Ti_3C_2 and Ti_3C_2-BTCA at 1.5 A g^{-1}

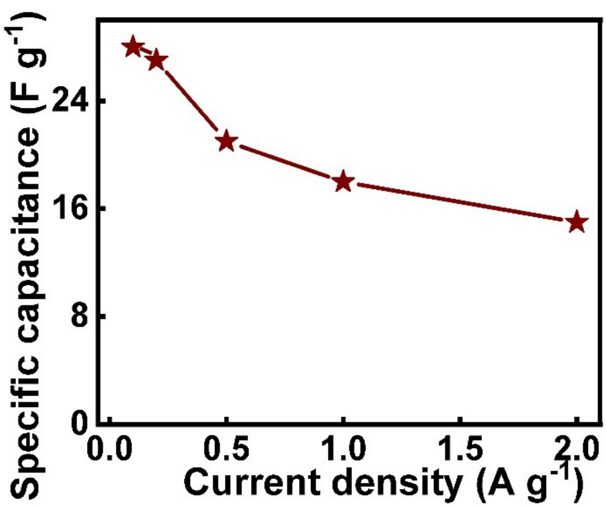

Figure S2. Specific capacity at different current densities of Ti_3C_2-BTCA||AC SIC.

The calculated specific capacities of Ti_3C_2-BTCA||AC SIC are 27.8, 24.2, 20.6, 17.7, 15.2, and 12 F g^{-1}, corresponding to 0.1, 0.2, 0.5, 1.0, 2.0 and 5.0 A g^{-1}, which can be obtained according to S6.

Table S1. Electrochemical performance y of Ti_3C_2-BTCA compared to previous reports

Anode material	Specific capacity (mAh g^{-1})	Max.current density (A g^{-1})	Cycle numbers	Reference
MoS_2/ $Ti_3C_2T_x$	162.7	1	100	6
Co_3C/MXene	105	2	100	7
N/O-C@TiO_2	165	1	1000	8
$V_4C_3T_x$ − C	128	1	100	9
Sb_2O_3 / Ti_3C_2	295	2	100	10
$Na_2Ti_3O_7$/ C	110	1	500	11
P-$Ti_3C_2T_x$	140	0.1	150	12
Ti_3C_2-BTCA	182.3	5	2000	**This work**

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