Supporting Information

Effect of Glycine Functionalization of 2D Titanium Carbide (MXene) on Charge Storage

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Characterizations.

XRD patterns of the samples were obtained using a Rigaku Smart Lab (Tokyo, Japan) with a Cu Kα radiation source (λ = 1.5406 Å).

The Raman spectra were recorded on Renishaw inVia spectrometer with a 632 nm laser as an excitation source (5% laser power).

The Fourier transform infrared (FTIR) spectra were collected by an ATR-FTIR spectrometer with a resolution of 4 cm⁻¹.

Cross-sectional images of d-Ti₃C₂Tₓ/glycine were obtained by using scanning electron microscopy (SEM, Zeiss Supra 50VP, Germany).

X-ray photoelectron (XPS) spectra were measured by a spectrometer (Physical Electronics, VersaProbe 5000, Chanhassen, MN) employing a monochromatic 100 μm Al Kα X-ray beam to irradiate the surface of the sample. Photoelectrons were collected by a 180° takeoff angle between the sample surface and the path to the analyzer. Charge neutralization was performed using a dual-beam charge neutralizer irradiating low-energy electrons and an ion beam to avoid shift in the recorded binding energy. High-resolution spectra were taken at a pass energy of 11.75 eV with a step size of 0.05 eV. The binding energy scale of all XPS spectra was referred to the Fermi-edge (E_F), which was set to a binding energy of zero eV. The powders were placed on a double-sided
tape. The quantification using the obtained core-level intensities and peak fitting of the core-level spectra was performed using a software package (CasaXPS Version 2.3.16 RP 1.6).

**Electrochemical tests**

All electrochemical measurements were performed in a 3-electrode configuration. As-prepared d-Ti$_3$C$_2$T$_x$/amino acid freestanding films with a thickness of ~4 μm served as a working electrode, over-capacitive activated carbon film was used as a counter electrode, glassy carbon electrodes were used as current collectors and Ag/AgCl served as a reference electrode. Activated carbon electrodes composition was 90 wt. % of YP-50 activated carbon (Kuraray, Japan), 5 wt. % of carbon black and 5 wt. % of polytetrafluoroethylene.

**Calculations of capacitance of electrode**

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C = (\int j \, dV)/(s \, V) \, [\text{F} \, \text{g}^{-1}]
\]

where \( C \) is gravimetric capacitance of electrode [F g\(^{-1}\)], \( j \) is current density [A g\(^{-1}\)], \( s \) is scan rate [V/s], \( V \) is voltage window [V].
Figure S1 Top views of the adsorption configurations
Figure S2 Thermogravimetric analysis of pristine Ti$_3$C$_2$Tx and Ti$_3$C$_2$Tx/glycine hybrid samples. We set 450 °C as the cut-off temperature, as oxidation of Ti$_3$C$_2$Tx beyond this temperature leads to an increase in the sample weight. The weight loss of d-Ti$_3$C$_2$Tx is due to trapped water between its layers. We used difference between the weight loss of d-Ti$_3$C$_2$Tx/glycine hybrid and pristine d-Ti$_3$C$_2$Tx to determine the glycine content, which is ~4.65%, assuming the same content of water and other adsorbed species in both samples.
Figure S3 Predicted interlayer spacing for Ti$_3$C$_2$O$_2$.

Figure S4 Three possible configurations (two parallel configurations and one vertical configuration) of water intercalated Ti$_3$C$_2$O$_2$: Two parallel configurations: two hydrogen atoms of H$_2$O point to two different oxygen atoms of Ti$_3$C$_2$O$_2$ surface; two hydrogen atoms of H$_2$O point to the same oxygen atom.
Figure S5 Rate performance and capacitance retention for pristine d-Ti$_3$C$_2$T$_x$, d-Ti$_3$C$_2$T$_x$/glycine and d-Ti$_3$C$_2$T$_x$/leucine samples. The leucine molecule is much larger than glycine. Therefore, it occupies more reactive sites of MXene, resulting in a low capacitance.