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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-$Ti_3C_2T_x$/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-$Ti_3C_2T_x$/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

$C = (\int j \, dV)/(s\ V)$ [F 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].

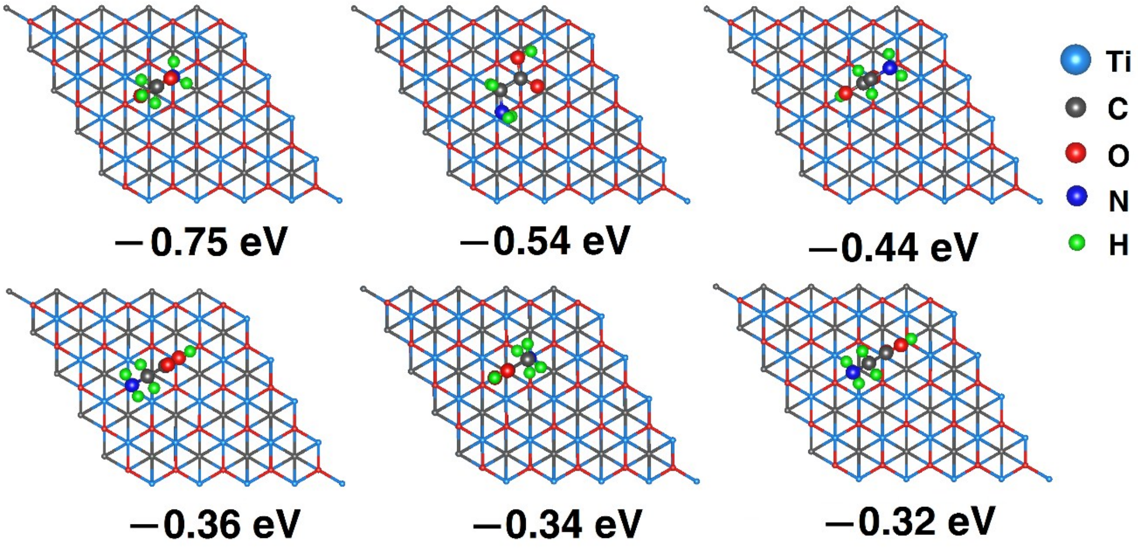

Figure S1 Top views of the adsorption configurations

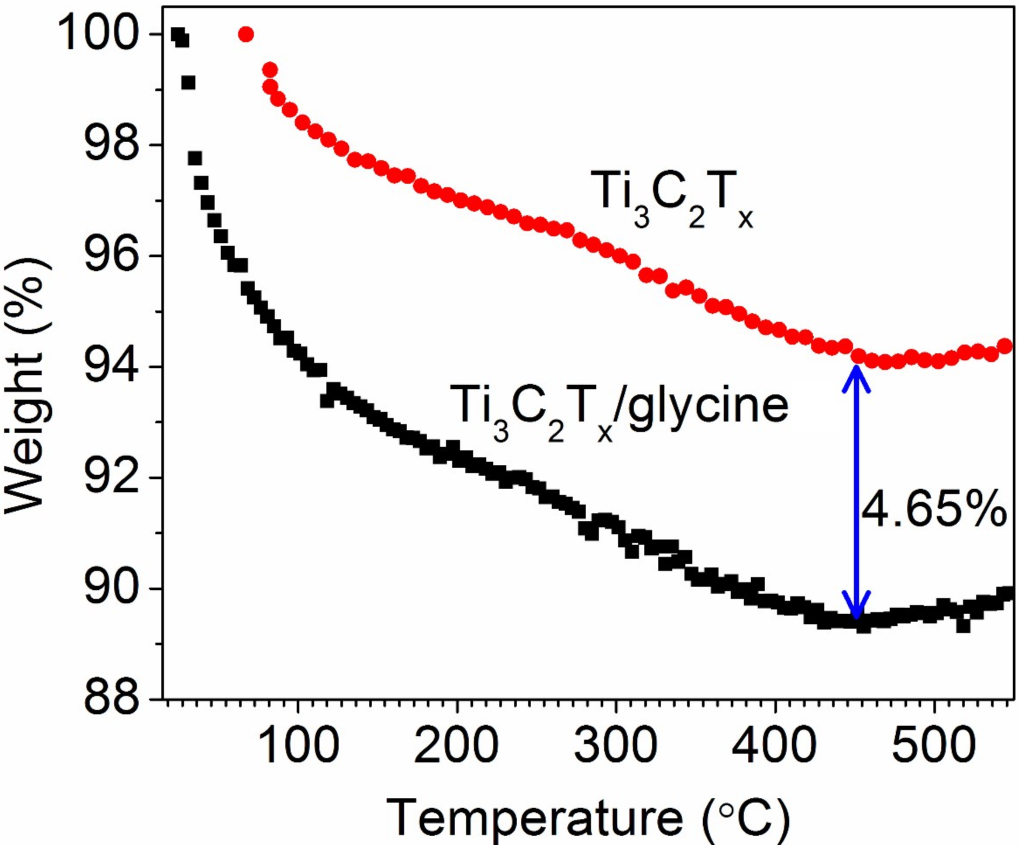

Figure S2 Thermogravimetric analysis of pristine $Ti_3C_2T_x$ and $Ti_3C_2T_x$/glycine hybrid samples. We set 450 °C as the cut-off temperature, as oxidation of $Ti_3C_2T_x$ beyond this temperature leads to an increase in the sample weight. The weight loss of d-$Ti_3C_2T_x$ is due to trapped water between its layers. We used difference between the weight loss of d-$Ti_3C_2T_x$/glycine hybrid and pristine d-$Ti_3C_2T_x$ to determine the glycine content, which is ~4.65%, assuming the same content of water and other adsorbed species in both samples.

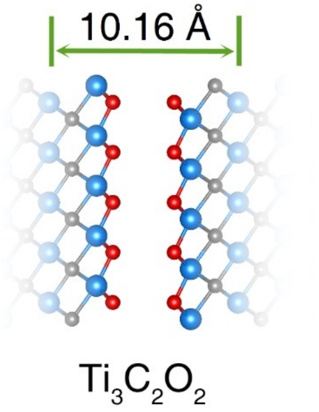

Figure S3 Predicted interlayer spacing for $Ti_3C_2O_2$.

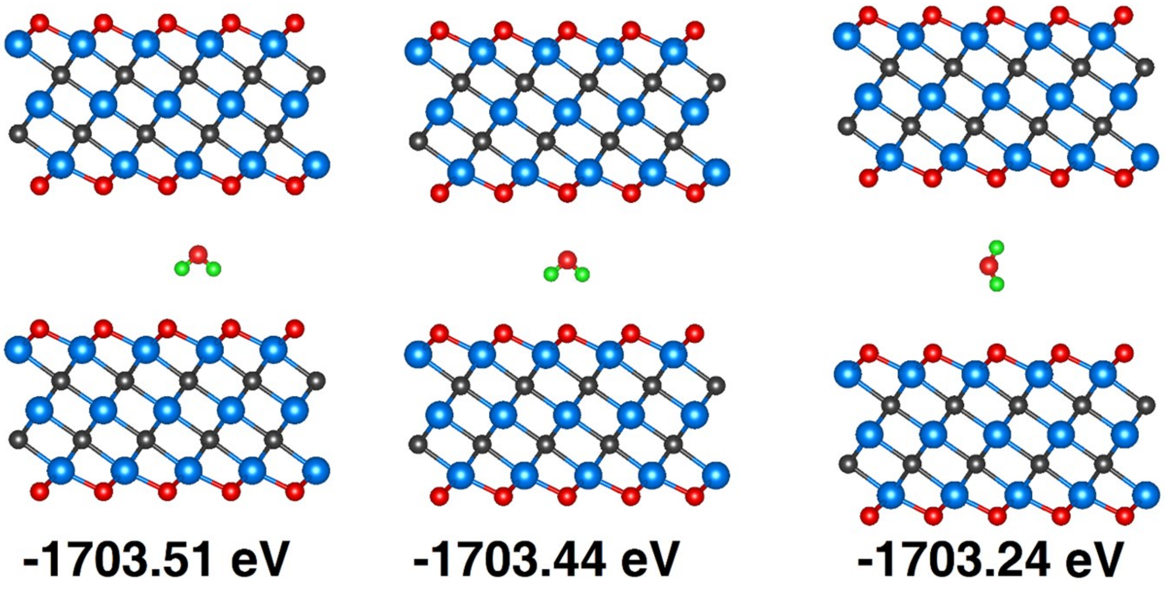

Figure S4 Three possible configurations (two parallel configurations and one vertical configuration) of water intercalated $Ti_3C_2O_2$.Two parallel configurations: two hydrogen atoms of H_2O point to two different oxygen atoms of $Ti_3C_2O_2$ surface; two hydrogen atoms of H_2O point to the same oxygen atom.

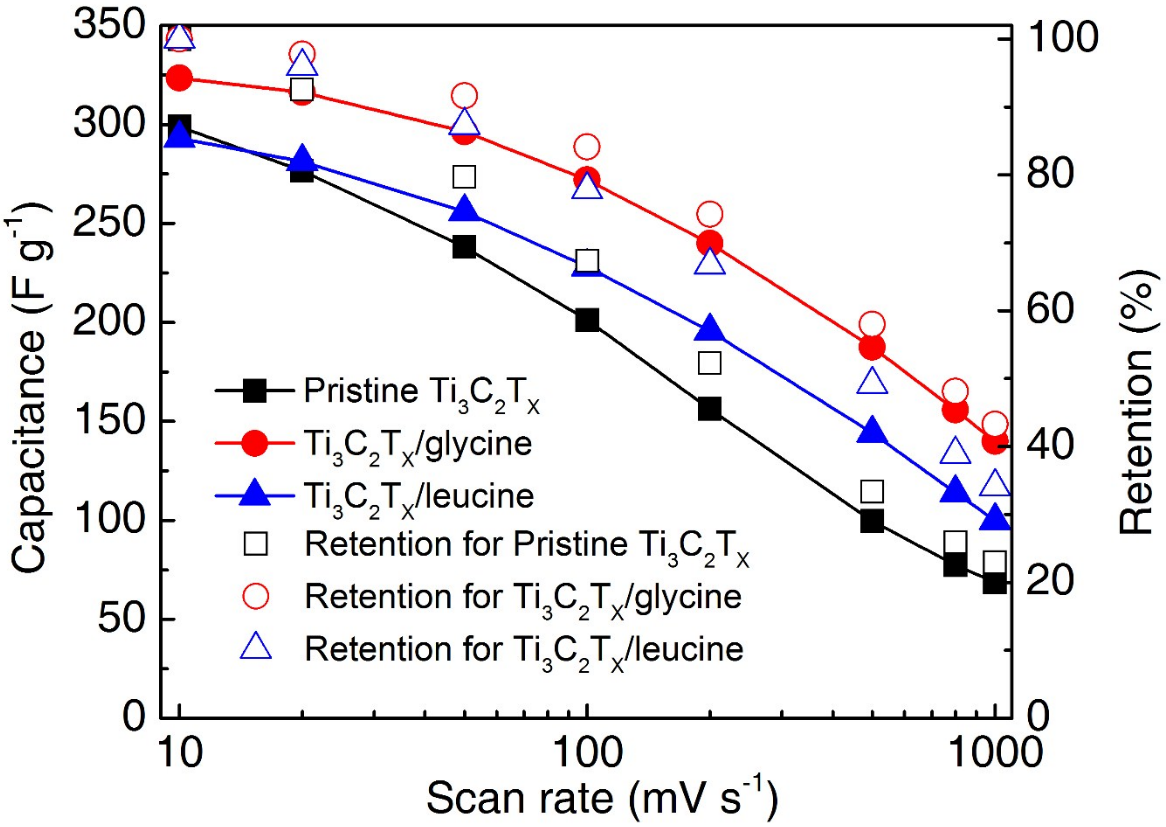

Figure S5 Rate performance and capacitance retention for pristine d-$Ti_3C_2T_x$, d-$Ti_3C_2T_x$/glycine and d-$Ti_3C_2T_x$/leucine samples. The leucine molecule is much larger than glycine. Therefore, it occupies more reactive sites of MXene, resulting in a low capacitance.