Supplementary Information

Understanding the Effect of Sodium Polyphosphate on Improving the Chemical Stability of $Ti_3C_2T_z$ MXene in Water

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The kinetics of degradation of $Ti_3C_2T_z$-Air, $Ti_3C_2T_z$-Ar, and $Ti_3C_2T_z$-PP samples are shown in Figure 2. The data were fit by the corresponding exponential growth functions:

$$A(t) = 60133.1 - 59536.6 \cdot e^{-\left(\frac{t}{120.6}\right)}$$ for $Ti_3C_2T_z$-Air

$$A(t) = 54881.6 - 53657.1 \cdot e^{-\left(\frac{t}{182.4}\right)}$$ for $Ti_3C_2T_z$-Ar

$$A(t) = 10160.7 - 9653.2 \cdot e^{-\left(\frac{t}{88.4}\right)}$$ for $Ti_3C_2T_z$-PP

The chemical reactions of MXene oxidation and hydrolysis are represented by the equations separately:

hydrolysis of $Ti_3C_2O_2$ MXene

$Ti_3C_2O_2+4H_2O=3TiO_2+2CH_4$ (1)

oxidation of $Ti_3C_2O_2$ MXene

$2Ti_3C_2O_2+7O_2=6TiO_2+2CO+2CO_2$ (2)

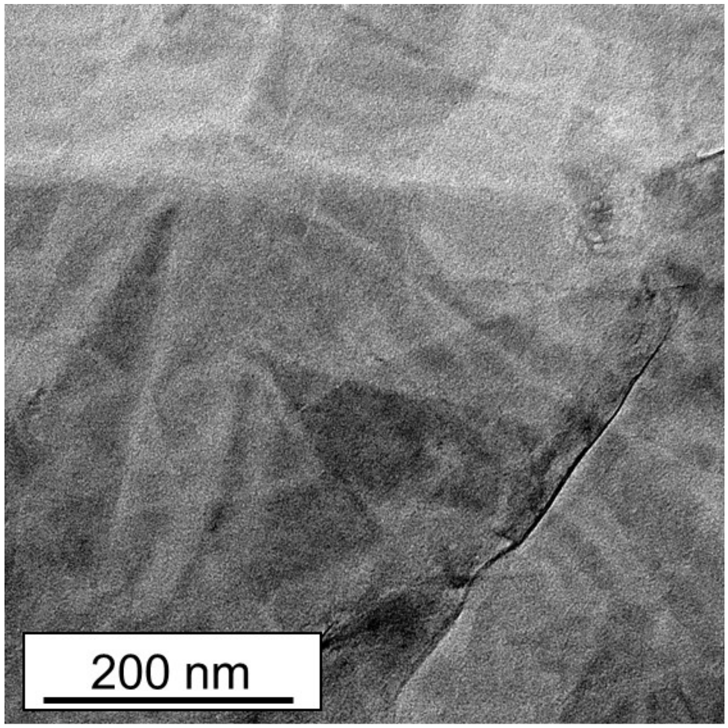

Fig. S1. TEM image of freshly made $Ti_3C_2T_z$ MXene flakes.

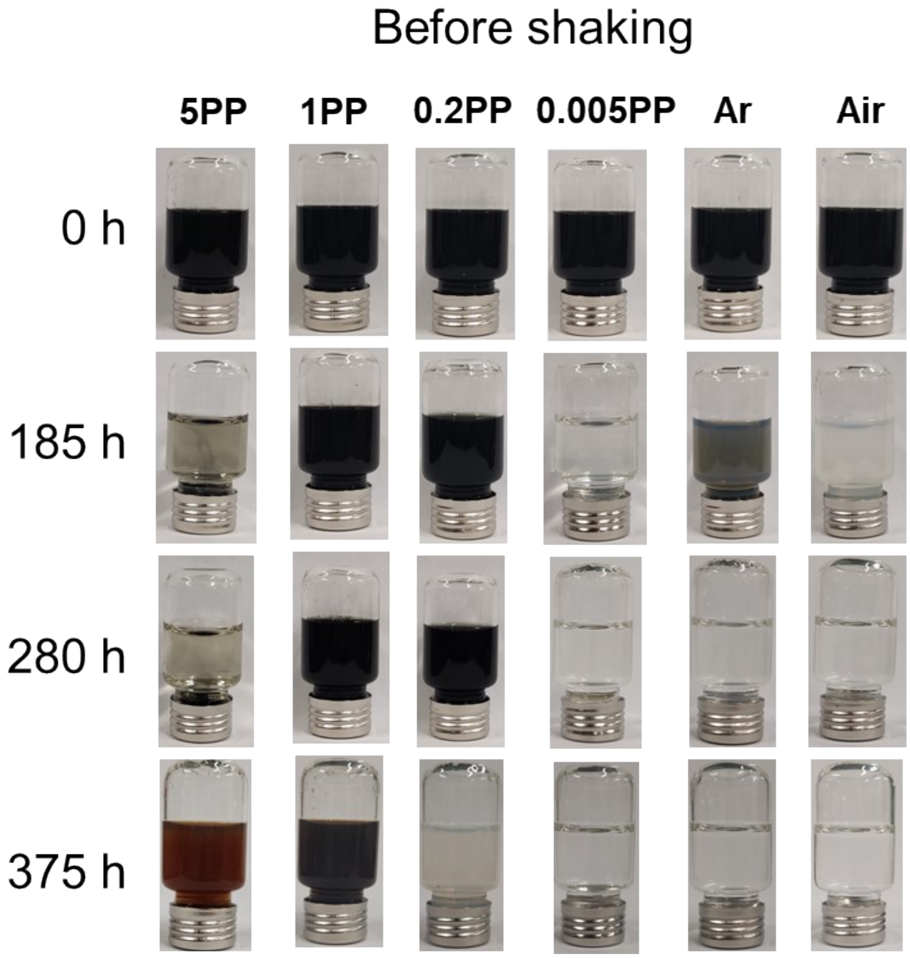

Fig. S2. Visual observations of $Ti_3C_2T_z$ MXene in different environments over time (before shaking).

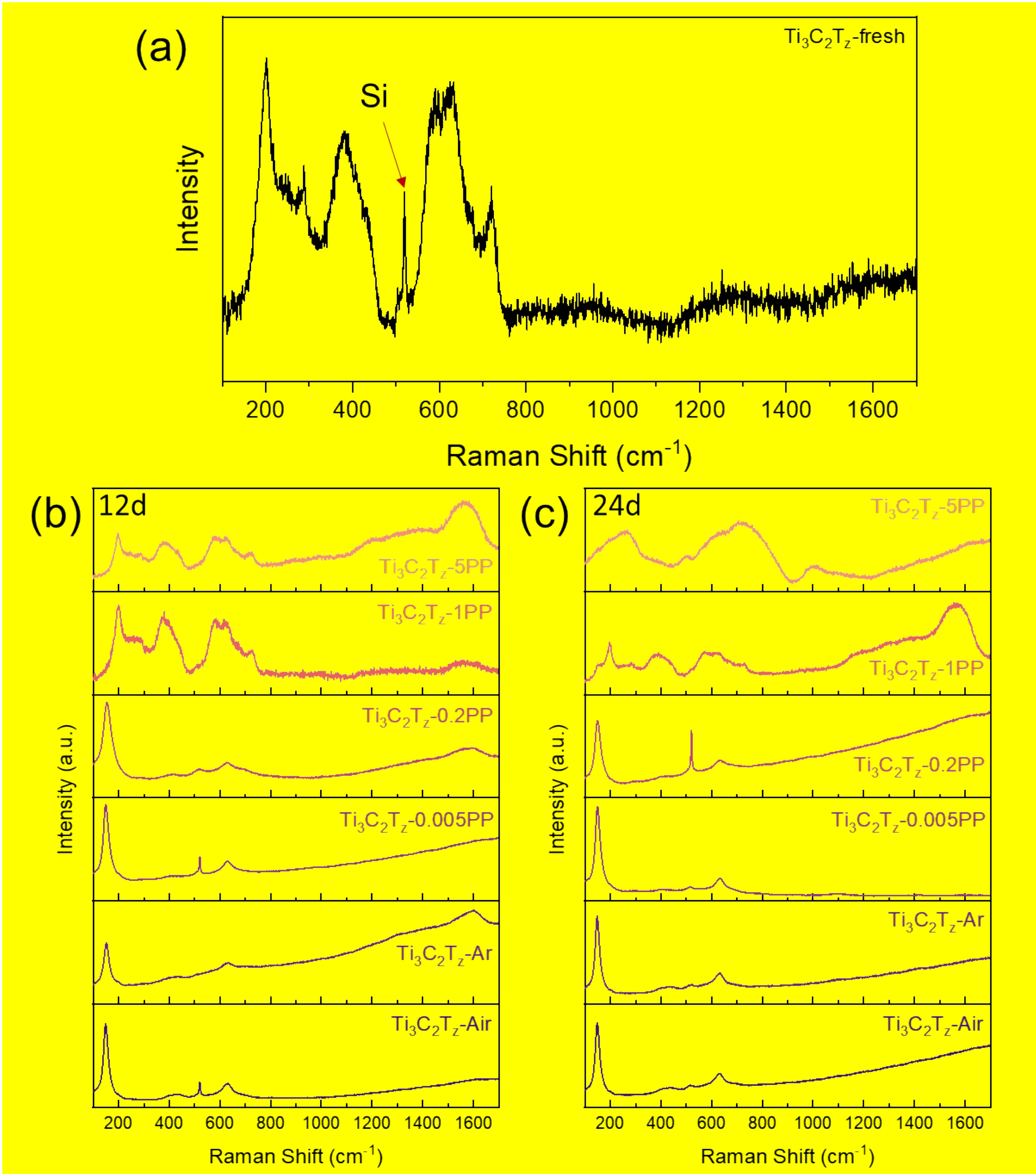

Fig. S3. Raman spectra of (a) fresh $Ti_3C_2T_z$ MXene, (b) $Ti_3C_2T_z$ MXene in different environments after 12 days, and (c) $Ti_3C_2T_z$ MXene in different environments after 24 days. All samples were stored in a 70 ^oC oven. The peaks at ~520 cm^{-1} apparent in some spectra are reflecting the signal from the Si wafer underneath the samples.

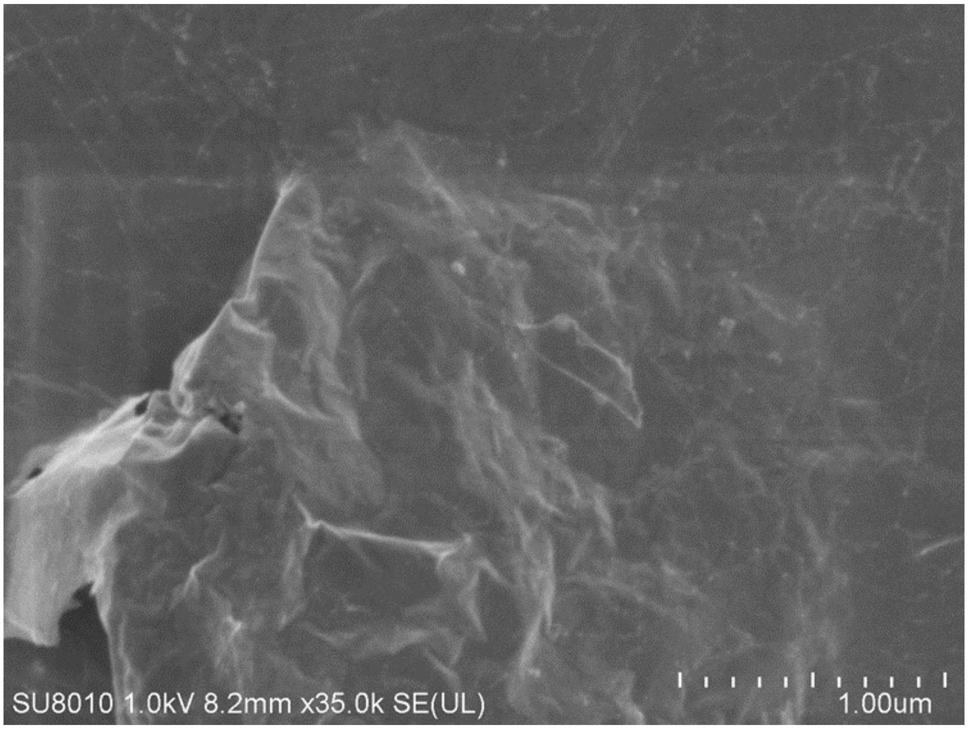

Fig. S4. SEM image of freshly made $Ti_3C_2T_z$ MXene film.

Assuming a MXene sheet with lateral dimensions of 0.8 μm length by 0.5 μm width

Perimeter

$p = 2 \times 0.8 + 2 \times 0.5 = 2.6\ \mu m$

Assuming sodium polyphosphate (PP) chain length ≈ 6 Å (this distance was calculated from the distance between the 1st and 3rd P atom)

Number of PP molecules needed to cap all edges of 1 MXene sheet

= 2.6/0.0006 ≈ 4333 molecules or ≈ 7.2×10^{-21} moles of PP

Volume of 1 MXene sheet assuming 0.001 μm (1 nm) thickness

$V = 0.8 \times 0.5 \times 0.001 = 4 \times 10^{-4}\ \mu m^3$

Density of MXene

$\approx 4.93 \frac{g}{cm^3} \approx 4.93 \times 10^{-12} \frac{g}{\mu m^3}$ (density of MXene was assumed to be same as the density of cubic TiC)

Mass of 1 MXene sheet

$= 4.93 \times 10^{-12} \frac{g}{\mu m^3} \times 4 \times 10^{-4}\ \mu m^3 = 1.9 \times 10^{-15}\ g \approx 2 \times 10^{-15} g$

Therefore 7.2×10^{-21} moles of PP are needed per $2 \times 10^{-15} g$ of MXene

= 3.6×10^{-6} moles of PP per g of MXene

≈ 0.0015 g of PP/ MXene sheet (Molar mass of PP = 367.9 g/mol)

As MXene sheet is ~1 nm thick and PP molecule thickness ≈ 0.3 nm (maximal distance between 2 O atoms connected to the same P atom) ≈ 3 PP molecules also need to be stacked vertically along a MXene sheet edge as well for complete coverage.

≈ 0.0015 $\times 3 \approx 0.005\ g$ of PP per g of MXene

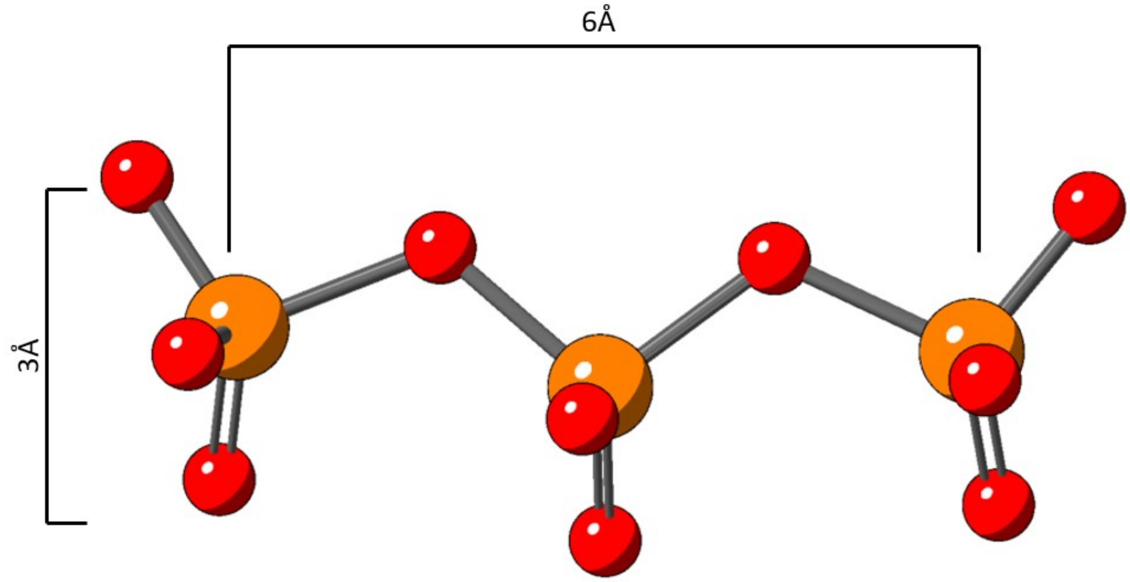

Fig. S5. Repeating unit of polyphosphate.