## SUPPLEMENTARY INFORMATION

## $Ti_{n+1}C_n$ MXene with fully saturated and thermally stable Cl terminations

J. Lu<sup>1</sup>, I. Persson<sup>1</sup>, H. Lind<sup>1</sup>, J. Palisaitis <sup>1</sup>, M. Li<sup>2</sup>, Y. Li<sup>2</sup>, K. Chen<sup>2</sup>, J. Zhou<sup>1,2</sup>, S. Du<sup>2</sup>, Z.

Chai<sup>2</sup>, Z. Huang<sup>2</sup>, L. Hultman<sup>1</sup>, P. Eklund<sup>1</sup>, J. Rosen<sup>1</sup>, Q. Huang<sup>2</sup>, and P. O.Å. Persson<sup>1</sup>

<sup>1</sup> Thin Film Physics Division, Department of Physics, Chemistry and Biology (IFM), Linköping University, SE-581 83 Linköping, Sweden

<sup>2</sup> Engineering Laboratory of Advanced Energy Materials (FiNE Lab.), Ningbo Institute of Industrial Technology, Chinese Academy of Sciences, Ningbo, Zhejiang, 315201, China

Corresponding author: per.persson@liu.se



Figure S1. Electron diffraction pattern obtained from the multilayer particle shown in fig 1b



Figure S2. Schematic description of the difference between fcc and hcp sites for a  $M_3X_2$ structure in a) cross-section and b) plan-view. The fcc site is positioned directly above an M atom of the middle layer (bottom layer in an  $M_2X$  structure), while an atom in the hcp site is positioned directly above the nearest X atom.



Figure S3. EDX spectra obtained from the Ti2CCl2 and Ti3C2Cl2 structures. The spectra are normalized against the Cl-K peak, which clearly shows a  $\sim$ 50 % increase in the Ti-K peak from the Ti2CCl2 to the Ti3C2Cl2 structure. The apparent differences at low energies are attributed to contributions from the supporting lacey carbon and from TiO2 particles.



Figure S4. Formation energy and optimum lattice parameters for Cl-terminated  $Ti_2C$  and  $Ti_3C_2$  with the terminations residing on AA - fcc sites (top and bottom surfaces), AB - fcc (top surface) and hcp (bottom surface) sites as well as BB - hcp sites (top and bottom surface). For  $Ti_3C_2$  the TT - atop configuration was also found to be stable.



Figure S5. Phonon dispersion relations for  $Ti_2CCl_2$  in a) and b) and for  $Ti_3C_2Cl_2$  in c) and d). The Cl terminations are is fcc coordinated in a) and c) while they are hcp coordinated in b) and d). All phonon branches are real, indicating that all structures are stable. The integrated density of states are shown to the right of the phonon dispersions.



Figure S6. Low magnification cross-sectional STEM image of the as heated  $Ti_3C_2Cl_X$  MXene, exhibiting local dark spots. The appearance suggests local porosities in the otherwise preserved MXene structure.

	Bond length	Planar spacing
(Ti <sub>2</sub> C) Ti-Cl	2.5091 Å	1.6766 Å
(Ti <sub>2</sub> C) Ti-C	2.1609 Å	1.0885 Å
(Ti <sub>3</sub> C <sub>2</sub> ) Ti1-Cl	2.5086 Å	1.7022 Å
(Ti <sub>3</sub> C <sub>2</sub> ) Ti1-C1	2.1131 Å	1.0341 Å
(Ti <sub>3</sub> C <sub>2</sub> ) Ti2-C1	2.2320 Å	1.2594 Å

Table S1. Calculated bond lengths and planar spacings for the fcc coordinated Cl terminatedMXenes. See schematic in S3 for notaation of atoms.