How the constant discovery of new 3D MAX phases ensures the expansion of the 2D MXene family

A. Champagne
O. Chaix-Pluchery, T. Ouisse, D. Pinek, I. Gélard, L. Jouffret, J. Rosen, M.W. Barsoum, J.-C. Charlier

MODL department, Institute of Condensed Matter and Nanosciences, UCLouvain, 1348 Louvain-la-Neuve, Belgium

aurelie.champagne@uclouvain.be

MAX phases, with formula $M_{n+1}AX_n$, are layered ceramics composed of two-dimensional (2D) $M_{n+1}X_n$ sheets separated by A layers [Fig.1, 2(a)], where M represents an early transition metal, A an element from groups 13 to 16, X either a carbon or a nitrogen atom, and *n* varies from 1 to 3 [1].
In 2011, a new family of 2D materials, called MXenes (Fig.1), was discovered, resulting from the selective etching of A layers from the parent MAX phases [2]. Most MXenes exhibit a unique combination of excellent physical and chemical properties [3]. Thanks to their versatile chemistry and the control of their surface terminations, MXene is now the largest 2D family competing in an impressive number of applications.
Recently, a new route to increase the elemental combination and to optimize MXene performance was proposed, consisting in the addition of a fourth element to the parent MAX phase. Historically, most MAX phase alloys existed as random solid solutions. In 2014, out-of-plane ordered quaternary MAX phases (*o*-MAX) [Fig.2(b)] were discovered [4]. In 2017, in-plane ordered quaternary MAX phases (*i*-MAX) [Fig.2(c)] were theoretically predicted and successfully synthesized with the formula $(M^1_{2/3}M^2_{1/3})_2AlC$ where M^1 and M^2 are two metals ordered in-plane [5,6]. Recently, the existence of rare-earth containing *i*-MAX phases with the chemical formula $(M_{2/3}RE_{1/3})_2AlC$ was revealed [7], and similar layered family with stoichiometry $M_4RE_4Al_7C_3$ [Fig.2(d)] was simultaneously discovered and found to be ferromagnetic [8]. Since all these new MAX phases contain aluminum, their conversion to 2D MXenes should be fairly straightforward.

The introduction of these different classes of MAX phases and their 2D counterparts, MXenes, will be followed by a discussion on their respective structural, electronic, and vibrational properties obtained both from *ab initio* calculations and experimental characterization techniques.

References

[1] M.W. Barsoum, Progress in Solid State Chemistry 28 (2000), 201
[2] M. Naguib, Adv. Materials 26 (2014), 992
[3] M.R. Lukatskaya, Nature Comm. 7 (2016), 1
[4] Z. Liu, Acta Materialia 73 (2014), 186
[5] Q. Tao, Nature Communications 8 (2017), 1
[6] M. Dahlqvist, Science Advances 3 (2017)
[7] Q. Tao et al., submitted (2019)
[8] Q. Tao, Phys. Rev. Materials 2 (2018) 114401

Figures

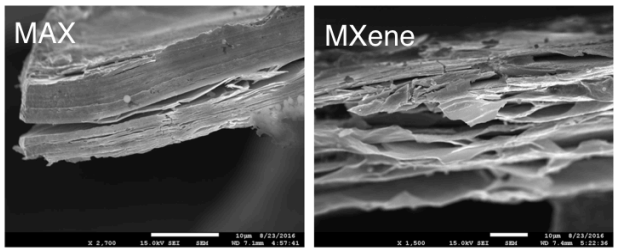

Figure 1: SEM images of a 3D MAX phase and the corresponding 2D MXene, after etching.

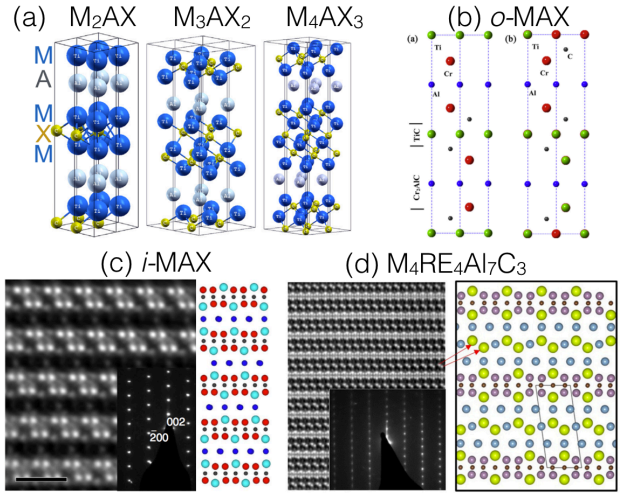

Figure 2: Atomic structures of different MAX systems, with STEM images for the last two.