Expanding the family of MAX phases: Synthesis of exotic layered solids

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Ternary carbides, nitrides and carbonitrides that belong to the family of MAX phases not only possess a unique set of properties (combining metallic and ceramic characteristics), they are also the precursors for their two-dimensional siblings, MXenes. MAX phases are structurally and chemically diverse and they encompass more than 150 members, many more solid solutions and a plethora of predicted compounds that have not been synthesized yet. They typically crystallize in a hexagonal structure with alternating layers of M_6X octahedra (*M* = early-to-mid transition metals, *X* = C and/or N) and the *A*-element (*A* = main group element or late transition metal). According to the general chemical formula $M_{n+1}AX_n$ (*n* = 1, 2, 3), "211", "312" and "413" MAX phases possess *n* (1, 2, 3) M_6X layers (2, 3 and 4 *M*-layers) between the *A*-layers, respectively [1].

A variant of the "211" MAX phase structure (left in Fig. 1) is the highly related "221" structure (right in Fig. 1) that crystallizes in the same hexagonal space group, $P6_3/mmc$, but features 2 *A*-element layers with the *A*-element stacked on top of one another, between the octahedral layers of *M* and *X*. What is very interesting is that only two compounds that adopt this double-*A* MAX phase structure have been synthesized: Mo_2Ga_2C [2] as a thin film and bulk and Ti_2Au_2C [3] as a thin film. V_2Ga_2C [4] has been theoretically predicted to be stable, however, has not been synthesized. "221" phases are structurally very interesting, but they also serve as a precursor of 2D MXenes. For example, MXene Mo_2CT_x can only be synthesized from "221" Mo_2Ga_2C (through HF-etching) and not from the "211" MAX phase Mo_2GaC.

In this talk, I will focus on the transition between "221" Mo_2Ga_2C and the fully exfoliated MXene version Mo_2CT_x using Lewis acids as the etchant. Besides the chemistry of these systems and transitions, I will discuss the structure of the compounds with varying Ga-content. I will further highlight additional "more exotic" MAX phases and MXenes that we investigate in our group, such as P-containing MAX phases and "higher" MXenes, such as $(Mo/V)_5C_4T_x$.

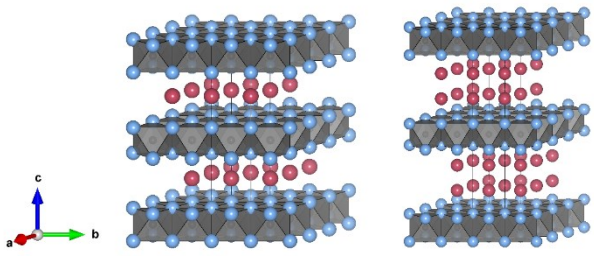

Fig. 1. Crystal structure of a 211 MAX phase (left) and a "221 MAX-like" phase (right). Blue: Mo, grey: C, red: Ga

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