First-principles study on mechanical and electronic properties of novel MAX phases

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MAX phases adopt crystal structures displayed in Figure 1 and show highly unusual mechanical, thermal, and electronic properties. While they conduct heat and electricity like metals, they are elastically stiff, strong, brittle, and heat-tolerant like ceramics. Some of the MAX phases kink and delaminate during deformation, many are resistant to chemical attack, readily machinable, and thermal shock, damage tolerant, and sometimes fatigue, creep, and oxidation resistant. Therefore, these systems attract great interest from point of view of industrial applications, including nuclear industries and renewable energy [2-4].

In this project, you will use first-principles electronic structure computational codes to simulate mechanical and electronic properties of potential new MAX phases and thus to guide the search for new members of the MAX family with most desired characteristics.

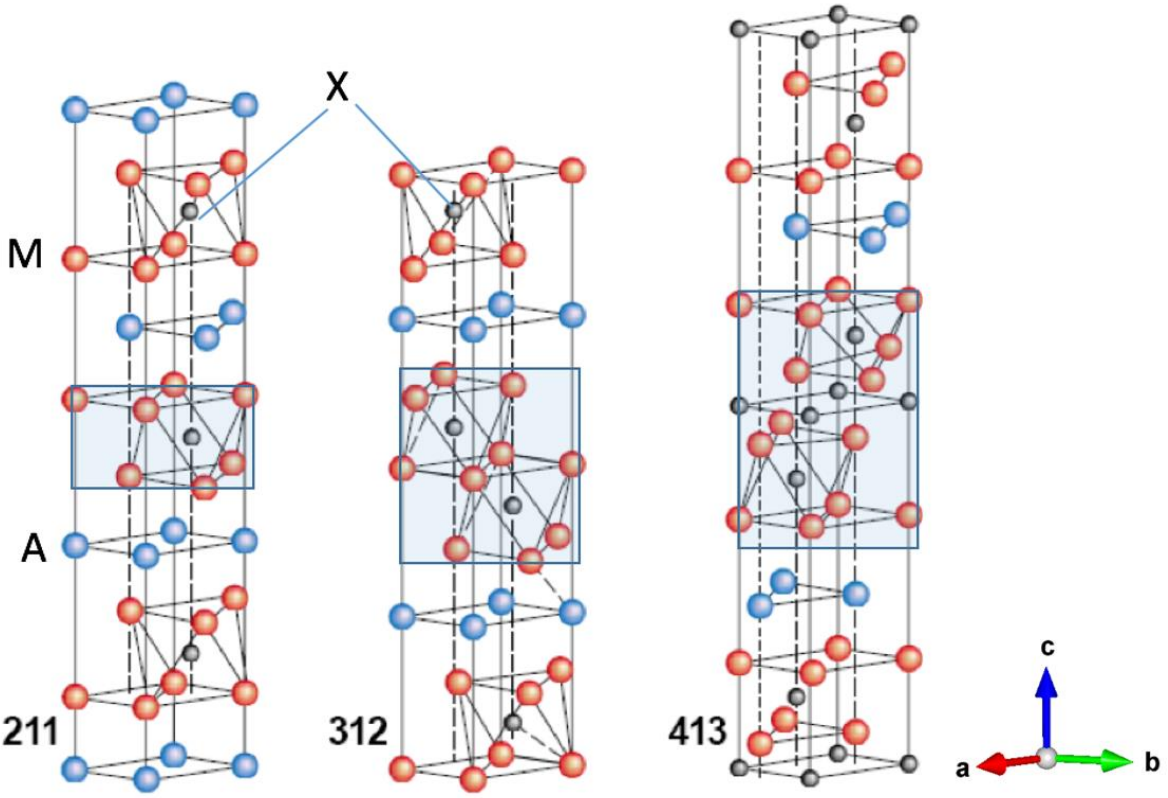

Figure 1: Crystal structures of MAX phases, i.e. layered hexagonal compounds with the chemical formula Mn+1AXn, where 'M' corresponds to an early transition metal, 'A' corresponds to an A-group element, 'X' corresponds to either carbon or nitrogen, and n=1, 2 or 3 (taken from [1]).

[1] Grey, V. (2014) $Ti_3SiC_2$and Ti_3AlC_2 Single Crystal Elastic Shear Modulus: Investigation via Inelastic Neutron Scattering and Computer Simulation. Newcastle University.

[2] Barsoum, M.W. (2000) 'The $M_{n+1}AX_n$ phase: a new class of solids; thermodynamically stable nanolaminates', Progress in solid state chemistry **28**, 201.

[2] Sun, Z.M. (2011) 'Progress in research and development on MAX phases: a family of layered ternary compounds', International Materials Reviews **56**, 143.

[3] Radovic, M. and Barsoum, M.W. (2013) 'MAX phases: Bridging the gap between metals and ceramics', American Ceramic Society Bulletin **92**, 20.

[4] Gonzalez-Julian, J. (2020) 'Processing of MAX phases: From synthesis to applications', Journal of the American Ceramic Society **104**, 659.