Decoding the Etching Protocols for Conversion of MAX Phases into 2D MXene structures

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Abstract

MXenes, a group of 2D materials with layers of transition metal carbides/nitrides/borides, and hold significant potential in energy storage, catalysis, and a wide range of applications. Synthesis of MXenes typically involves etching A-layer atoms from MAX phases using acid, alkali, or molten salt etchants [1], however the atomistic mechanisms behind this process are not fully understood [2-4]. We used ab-initio calculations to explore the thermodynamic drive and defect formation energies for 11 MAX phases; Ti_2AlC, Ti_3AlC_2, Ti_2AlN, Ti_4AlN_3, Ta_2AlC, Ta_4AlC_3, Cr_2AlC, V_2AlC, V_4AlC_3, Nb_2AlC and Nb_4AlC_3. Contrary to conventional wisdom, we find that the etching mechanism is not limited by thermodynamic feasibility, and that the inability to synthesize many compositions is due to kinetic constraints. We demonstrate, as a proof of concept study, the applicability of defect engineering approach for development of etching protocols in the broader MXene compositional phase space to pave the way for accelerated and commercial scale MXene synthesis.

References

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Figures

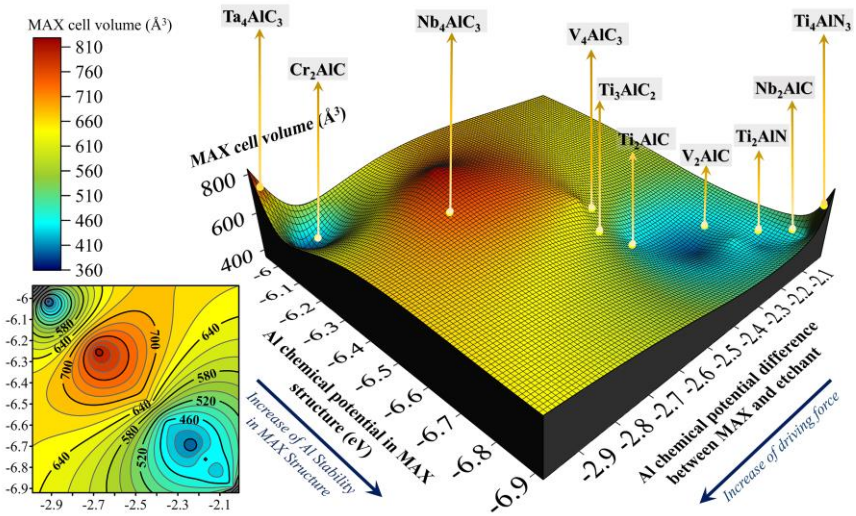

Figure 1: 3D representation of the etching driving force and its correlation with MAX cell volume, and Al chemical potential