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ABSTRACT

MXenes: Etching Kinetics and Ionic Transport in 2D Confinement

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MXenes are a family of two-dimensional (2D) early transition metal carbides, nitrides, oxycarbides, carbonitrides, and related structures with a general formula of $M_{n+1}X_nT_x$, where M is a transition metal, X is carbon or nitrogen (oxygen substitution is possible), T represents the surface terminations (O, OH, halogen, chalcogen, etc.), and n = 1—4 [1]. These materials are explored in various applications, such as energy harvesting and storage, water desalination, wireless communication, and photothermal therapy, because of their redox-active surfaces, high electrical conductivity, and plasmonic behavior. MXenes are typically produced by selective etching of MAX phases, which requires the removal of atomically thin metal (e.g., Al) layers connecting carbide or nitride lamellae. Knowing the etching kinetics allows one to predict the process time as a function of temperature, particle size, and other parameters. Our study of the kinetics of the MAX etching reaction for topochemical MXene synthesis led to the development of an empirical model for predicting the time necessary to produce MXene for any given input parameters [2]. Specifically, for Ti_3AlC_2 MAX, this kinetic model resulted in an apparent activation energy of about 55 kJ/mol. Transport in 2D slits between MXene layers is important not only during the material synthesis but also in many applications, such as electrochemical energy storage (batteries and supercapacitors) and water deionization. I'll discuss how the presence of ions affects water dynamics in 2D confinement [3] and the implications for numerous technologies.

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