Two-Dimensional Metal Nitride (Mn+1Xn) MXene: Synthesis, Characterization, and Potential Application as Energy Storage Materials

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Abstract : MXenes was known as potential candidates for a myriad of applications ranging from electrochemical energy storage materials (Batteries and supercapacitors), sensors, and electronic devices. Here I am proposing a new method to synthesize two dimensional metal nitride.

IndexTerms – Mxenes, metal nitride, 2D materials, energy storage

The energy crisis and environmental pollution have forced us to adopt electricity generated by renewable energies such as wind, solar, and water power. However, due to the intermittent nature of these renewable energies, it is imperative to develop energy storage devices for the more efficient utilization of renewable energies. MXenes, a family of 2D transition metal carbides and nitrides, was developed by a group of researchers from Drexel University have attracted extensive research attention for energy storage in the past years because of their unique physical and chemical properties[1]. Their general formula is $M_{n+1}X_nT_x$ (n = 1–3), where M represents an early transition metal (such as Sc, Ti, Zr, Hf, V, Nb, Ta, Cr, Mo and so on), X is carbon and/or nitrogen and T_x stands for the surface terminations (for example, as -O, -OH, and -F)[1].

MXenes was known as potential candidates for a myriad of applications ranging from electrochemical energy storage materials (Batteries and supercapacitors), sensors, and electronic devices etc.[2]. Among all the applications listed, most explored is their use in energy storage applications utilizing its ability to accommodate ions of various sizes between 2D layers, good electronic properties and large surface areas of MXenes. In Li-ion batteries, a steady-state capacity can be achieved when Li^+ ions are intercalated into MXenes. Moreover, Li^+ ions are predicted to diffuse quickly on the surface of MXenes, resulting in large storage capacity and outstanding high rate capability[2]. Similarly supercapacitors have attracted a lot of research interest due to the high power density, rapid charging/discharging rate and long cycle life, but compared with batteries, supercapacitors suffer from lower energy density. MXene-based materials are expected to be promising candidates for supercapacitors because of above-mentioned characteristics. In contrast to carbides and carbonitrides MXenes, nitride-based MXenes possess several advantages due to their higher electronic conductivity[3]. However, nitride-based MXenes remain unexplored due to the intricacy in the synthesis and due to their low stability in etchants such as HF[4].

Herein we propose the synthesis of metal nitrides (MXene) (Zr, V, Cr, Hf etc.) from its 3D counterpart (Max phase). MXenes can be prepared by selectively etching the reactive "X" layers in laminated nitrides Max phase. The synthesis conditions remarkably influence the properties of the final products and thus directly affect the performances of MXenes in their applications. The most commonly used method for the synthesis of MXene flakes is by LiF + HCl etching. However, this will results MXene have a larger lateral size without nanoscale defects[5]. Therefore, mild etching conditions are usually preferred to synthesize MXenes for energy storage applications[6]. However, a low concentration of HF or HF-containing salt and a short etching time may reduce the yield of the desired product. Therefore, the preparation conditions must be optimized to maximize the yield and application range of MXenes.

Thus through this proposal, we would like to explore various method to synthesize novel metal nitrides by adopting different approaches. The approaches are summarized below.

1. Reducing the MAX phase particle size by attrition or ball milling: Discrepancies in M-X bond energies for different MAX phases also require different etching conditions. For example, the larger Ti-Al bond energy in Ti_2AlC compared with the Nb-Al bond energy in Nb_2AlC resulted in extended etching time and increased HF concentration. This can effectively reduce the necessary etching time and/or HF concentration.
2. One step etching: Ammonium bifluoride, (NH_4HF_2), as an etchant instead of the hazardous HF. Its milder nature and concomitant intercalation of cations during the etching process render it more suitable for preparing delaminated MXenes as the etching and intercalation processes occur simultaneously.
3. Fluorine-free etching process: Using alkaline solution: Differing from the previous fluoride-containing acidic etching routes the surface terminations are only -OH and -O groups only will occur during this approach. This fluoride free method significantly reduces safety concerns and provides an alkali-etching strategy for exploring new MXenes.

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