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SYNTHESIS AND OPTICAL PROPERTIES OF 2D CARBIDES MXENES

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The family of two-dimensional (2D) transition metal carbides and nitrides, MXenes, has been expanding rapidly since the discovery of Ti₃C₂ MXene in 2011 [1]. More than 20 different MXenes have been synthesized, and the structure and properties of numerous other MXenes

have been predicted using density functional theory calculations [2]. Two-dimensional (2D) materials with a thickness of a few nanometers or less can be used as single sheets due to their unique properties or as building blocks, to assemble a variety of structures. MXenes properties can be tunable for a large variety of applications [3] that directly lead to their use for electromagnetic shielding [4], transparent conductors, light-to-heat energy conversion [5], new advanced lasers and photothermal therapy [6].

The 2D structure, combined with high electrical conductivity and good electronic coupling between the layers, resulted very high electromagnetic interference shielding efficiency of MXenes [4].

Research results showed that MXenes demonstrates an outstanding internal light-to-heat conversion efficiency (~100%) and show much more higher light absorption capability than other materials [5]. The 2D titanium carbide sheets show strong optical absorption in the near-infrared (NIR) around 800 nm. The performance of this material is comparable or even superior to that of state-of-the-art photo absorption materials, including gold-based nanostructures, carbon nanomaterials, and transition-metal dichalcogenides.

Unique optical and plasmonic properties have also been demonstrated, making the materials promising for photothermal therapy applications. Preliminary studies show that the titanium carbide sheets serve as an efficient photothermal agent against tumor cells [6].

Synthesis of MXene begins with etching with 10% wt. HF solution and/or a mixture of salts and acids at room temperature or slightly higher temperature the A-element atomic layers (for example, aluminum) in a MAX phase (for example, Ti₃AlC₂). After the etching is finished (complete removal of the A-element layers), washing must be applied to remove residual acid and reaction products (salts) and achieve a safe pH (~6). After the pH is increased to ~6, and intercalation of

large organic molecules and subsequent delamination completed, the multilayered MXene flakes or single nanosheets can be collected via vacuum-assisted filtration and then dried in vacuum [7].



Fig. 1. Pilot laboratory line with controlled parameters for MXene synthesis (up to 100 g per batch): 1 – computer control system; 2- Etching reactor for MXene synthesis; 3 – additional equipment for laboratory technological line.

MXenes can be deposited by spin, spray, or dip coating, painted or printed, or fabricated in a variety of ways. Synthesis conditions used to produce MXenes influence the resulting properties and thus are directly related to the performance of MXenes in their applications [7].

In the laboratory, researchers synthesize MXene in very small quantity (milligrams), and it is very difficult to repeat the synthesis conditions in order to obtain a material with the same repeatable properties.

For scaling up laboratory process and to obtain the material in larger quantities (up to 100 g per batch) of good quality with repeatable properties, a pilot laboratory line was developed [7] (Fig. 1), which allows to control the etching process and adjust its basic parameters - temperature, mixing speed, recording and storing all necessary data for analysis or to repeat the conditions during subsequent syntheses to obtain a MXene with repeatable properties.

In addition, since the acidic etching process is accompanied by the release of heat, a specially developed sealed reactor allows more secure synthesis, and also the computer control system provides the desired optimal synthesis temperature.

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