GROWTH OF MXENE BY CHEMICAL VAPOR DEPOSITION

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Two-dimensional (2D) materials based on transition metal carbides and nitrides, also known as MXenes, are a class of 2D materials that have seen exceptional development since their discovery in 2011. They show particular promise for electrochemical energy storage. Unfortunately, their synthesis is currently not sustainable because it requires a significant amount of energy as well as the use of toxic chemicals (e.g., HF). In this project, I propose to develop the synthesis of MXenes via chemical vapor deposition (CVD). The CVD synthesis of MXenes (Figure 1), first reported in 2023 [1], opens up entirely new possibilities for this class of materials. In addition to offering great versatility in the chemistry of the synthesized materials through the use of different precursors [2], CVD growth allows for a uniform halogenated surface chemistry and can be performed directly on a metallic—and potentially carbon-based—substrate, which is particularly well-suited for electrochemical energy storage. Controlling the growth parameters (e.g., precursors, temperature, growth time) as well as characterizing the materials will be the main challenges of this project.

The project will focus primarily on the synthesis of MXenes with the formula M_2CCl_2, whose morphology—including layer thickness, density, and structure—we will control. Several transition metals M (Ti, V, or Mo) will be studied. M_2CCl_2-type MXenes promise a higher theoretical energy density than $M_3C_2Cl_2$ MXenes, such as $Ti_3C_2Cl_2$, which are commonly used for electrochemical energy storage, but the poor chemical stability of Ti_2CCl_2 synthesized via conventional chemical methods (MAX phase etching in an acidic medium) prevents good electrochemical performance due to excessive structural defects. Their application as a negative electrode for sodium-ion batteries will be demonstrated in this thesis by combining them with hard carbon (HC) materials. These are commonly used in Na-ion batteries due to their high capacity, but they have limitations at high charging rates. The high conductivity of MXenes will help overcome this limitation. Hard carbon can prevent the restacking of MXene layers, which will improve ionic diffusion and stability during prolonged cycling. The pseudocapacitive or intercalation storage of MXenes, combined with the adsorption/insertion storage of HC, should result in a hybrid mechanism offering improved performance.

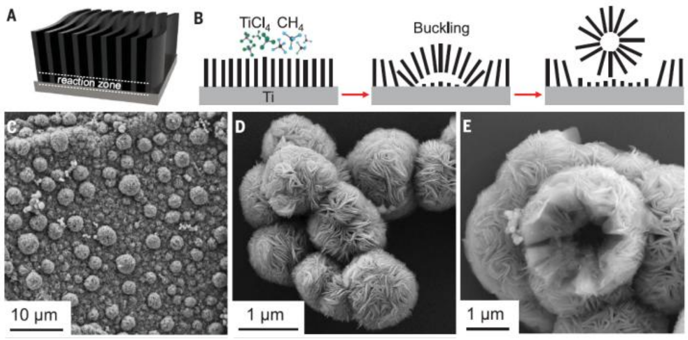

Figure 1 : (A-B) scheme of CVD growth of Ti_2CCl_2 MXene. (C-E) Scanning electron micrographs of CVD-grown MXene flakes. Adapted from reference [1].

[1] D. Wang *et al.*, "Direct synthesis and chemical vapor deposition of 2D carbide and nitride MXenes," *Science*, vol. 379, no. 6638, pp. 1242–1247, 2023.
[2] D. Wang *et al.*, "Molecular organohalides as general precursors for direct synthesis of two-dimensional transition metal carbide MXenes," *Nat. Synth. 2025*, pp. 1–9, 2025.