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Influence of Surface Terminations (–F, –OH, –Cl) on the Structural and Electrochemical Behavior of $Ti_3C_2T_x$ MXene

The rapid evolution of electrochemical energy storage and the growing environmental concerns demands advanced materials. MXenes, particularly Ti3C2 have been targeted to meet these demands due to their exceptional conductivity, layered structure, and tunable surface terminations. Generally, MXenes acquire surface terminations such as -OH, -O, -Cl, and -F after the etching process, which can be modified by post-synthesis treatment such as cleaning with ammonia solution (NH4OH). Herein, we study the effects of ammonia post-synthesis treatment on the structure and electrochemical performance of Ti3C2 MXene synthesized via in-situ HF etching. The aim is to understand how ammonia treatment influences the surface terminations, structure, and resulting electrochemical properties in both batteries and supercapacitors applications. Structural analysis using the SEM, EDX, and XRD revealed that ammonia hydroxide treatment effectively removes the residual fluoride (-F), chloride (-Cl), and aluminum (-Al) while preserving the layered structure of the MXene. XRD patterns further showed the eradication of (104) peak at ~39.0° 2θ for all samples, indicating the full conversion of Ti3AlC2 to Ti3C2, with no significant impurity signals as seen on the EDX data, corroborating SEM and EDX analyses. Electrochemical testing for supercapacitor application revealed that the CV curves of ammonia-treated MXene exhibited reduced current response and charge separation compared to the untreated sample, suggesting diminished pseudocapacitive behaviour and hence, lower capacitance. The GCD evaluation of both ammonia-treated and untreated samples showed nearly symmetrical curves, indicating good electrochemical reversibility. However, the ammonia-treated MXene had lower specific capacitance and decreased charge-discharge efficiency. On the contrary, it is reported that for battery systems the ammonia-treated MXene exhibits superior performance due to reduced -F termination that leads to enhanced ionic intercalation and lower charge-transfer resistance that benefits Li-ion insertion/extraction. NH4OH treatment also offers increased -O and -OH terminations promoting stronger chemical bonding while boosting capacity and cycling stability. The study has shown that ammonia treatment of Ti_3C_2 MXene detrimentally affects its electrochemical properties for supercapacitor application.

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