ISBN:
978-1-917892-15-5

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Lewis Acid Molten Salt-Derived MXene Electrodes: Dual Oxide Coating and Porosity Engineering for Advanced Energy Storage

Abstract: MXenes, a class of two-dimensional (2D) transition metal carbides and nitrides, offer significant potential for electrochemical energy storage applications due to their excellent electronic conductivity, tunable surface chemistry, and layered architecture. However, conventional synthesis using hydrofluoric acid (HF) is toxic and corrosive and possesses safety risks. Additionally, 2D MXenes experience limited ion transport and structural instability, hindering long-term performance. In this study, we present a 3D flower-like double transition metal MXene, Mo2Ti2C3Clx, featuring engineered in-plane mesoporosity, synthesized via a HF-free Lewis acid molten salt method combined with intercalation and freeze-drying. Controlling the molar ratio of Lewis acid to eutectic salts creates stable mesoporosity, preserved through freeze-drying. Molecular dynamics (MD) simulations show the effect of in-plane pore sizes on electrolyte transport, while density functional theory (DFT) calculations demonstrate that chlorine surface groups significantly lower Li-ion diffusion barriers. Electrochemical tests reveal that small-sized (2-5 nm) mesoporous Mo2Ti2C3Clx achieves a specific capacity of 324 mAh g-1 at 0.2 A g-1 and retains 97% capacity after 500 cycles at 0.5 A g-1, outperforming larger-pored (10 nm) and nonporous Mo2Ti2C3Clx variants. This work highlights a scalable strategy for creating mesoporous MXenes that enhance ion transport and structural stability, essential for next-generation highperformance energy storage systems.

Keywords: metal carbide, MXene, batteries, electrochemical, Lewis acid, porous electrode

Biography: Prof. Tan is the deputy director of the Department of Materials Science and Engineering and the director of the Guangdong Key Laboratory of Energy Conversion. In 1989, he obtained a PhD in Physics from Chinese Academy of Sciences. He then taught at the University of Science and Technology of China. From 1994 to 2018, he received PhD from the University of Illinois at Urbana-Champaign. Then, he entered the industry to study dielectric ceramics and polymers, energy storage materials, and filtration membrane technology for 20 years. He has published 120 papers and 60 issued patents.