

2D Carbides and Nitrides (MXenes) for Electrochemical Energy Storage

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The market and policy shift from use of fossil fuels to electricity for powering cars and future cities, has created an enormous demand for development of next generation energy storage devices that can meet such criteria as low manufacturing cost, scalability, long operating life, and high power and energy delivery. Discovery of new materials, design of electrode structures, cell components, and manufacturing processes are a key in meeting these targets by 2030. Nanomaterials, particularly, two-dimensional (2D) materials, are among promising candidates that can be used to address some of the ongoing challenges in manufacturing batteries and supercapacitors and enable devices with superior performance metrics and lower cost.^{1,2} Two-dimensional metal carbides and nitrides (MXenes) are a very large and yet quickly growing family of 2D materials with formula of $M_{n+1}X_nT_x$ where M is an early transition metal, X is carbon or nitrogen, and T_x refers to the surface terminations. Molecular dynamics and *ab initio* simulations, along with experiments, show that electronic, optical, and most importantly, electrochemical properties of MXenes distinguish them from other widely studied 2D materials. Chemical and electrochemical insertion of ions and molecules between the MXene layers allows modification of their properties, as well as electrochemical charge storage and harvesting, which use both, double-layer and redox mechanisms. The high electronic conductivity ($\sim 20,000 \text{ S cm}^{-1}$), redox active surfaces, cation intercalation in 2D slits, and rich chemistry of these materials with more than 50 different compositions reported, have enabled their use as charge storage hosts and building blocks of passive cell components in various types of energy storage devices.³ Freestanding, binder free films of $\text{Ti}_3\text{C}_2\text{T}_x$ are capable of ultra-high-rate pseudocapacitive charge storage in protic electrolytes delivering $\sim 400 \text{ F g}^{-1}$ (1500 F/cm^{-3}) at rates of up to 100 V s^{-1} and volumetric energy and power densities several times higher than conventional carbon based capacitive electrodes. MXenes can intercalate a variety of monovalent and multivalent cations from aqueous or non-aqueous electrolytes and, therefore, can be used as electrodes for emerging new battery chemistries. Their mechanical robustness and high conductivity expands their use as conductive additives in electrodes and also building blocks for conformal coatings to avoid dendrite growth in metal batteries. Yet, unlike most other 2D materials, synthesis and processing of MXenes is scalable and cost effective, and they can be processed in large batches from aqueous solution into various forms of powders, dispersions, and films. The combination of these properties and scalable synthesis, not only renders MXenes as interesting materials for academic research and development studies, but also as practical materials of choice for future charge storage applications.

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