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Discovery and Lab-scale Mechanistic Characterization of Selective Etched Metastable Materials for Electrochemical Energy Storage

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Lithium-ion batteries have revolutionized wireless electronics and are now transforming the automotive industry. The next level of adoption demands lower cost, safer supply chains, and higher energy density. New materials composed of more abundant elements can tackle these challenges and potentially provide better performance. However, new material discovery for energy storage faces two challenges: first, there is limited materials space after decades of exploration; second, bringing a material from discovery to market is slow, as it takes a long time to understand and optimize a material for energy storage. In this talk, we address these challenges from the synthesis and characterization perspectives. Although the materials obtained from direct synthesis methods have been largely explored, significant materials space is available via indirect methods, such as selective etching, which can lead to thermodynamically metastable materials with intriguing properties, such as MXenes (2D transition metal carbides and nitrides). Here, we show this method can be applied to oxides to discover new materials for energy storage, such as hydrogen tungstate. To reduce the time required to understand and optimize these materials, we developed a simple and easily accessible in situ ultraviolet-visible (UV-Vis) spectroscopy method to distinguish battery-type, pseudocapacitive, and electrical double-layer charge storage processes. It also allows us to quantify the electron transfer number during energy storage, which typically requires synchrotron-based X-ray absorption spectroscopy. These advances in synthesis and characterization can aid in more efficient materials discovery for energy resilience.